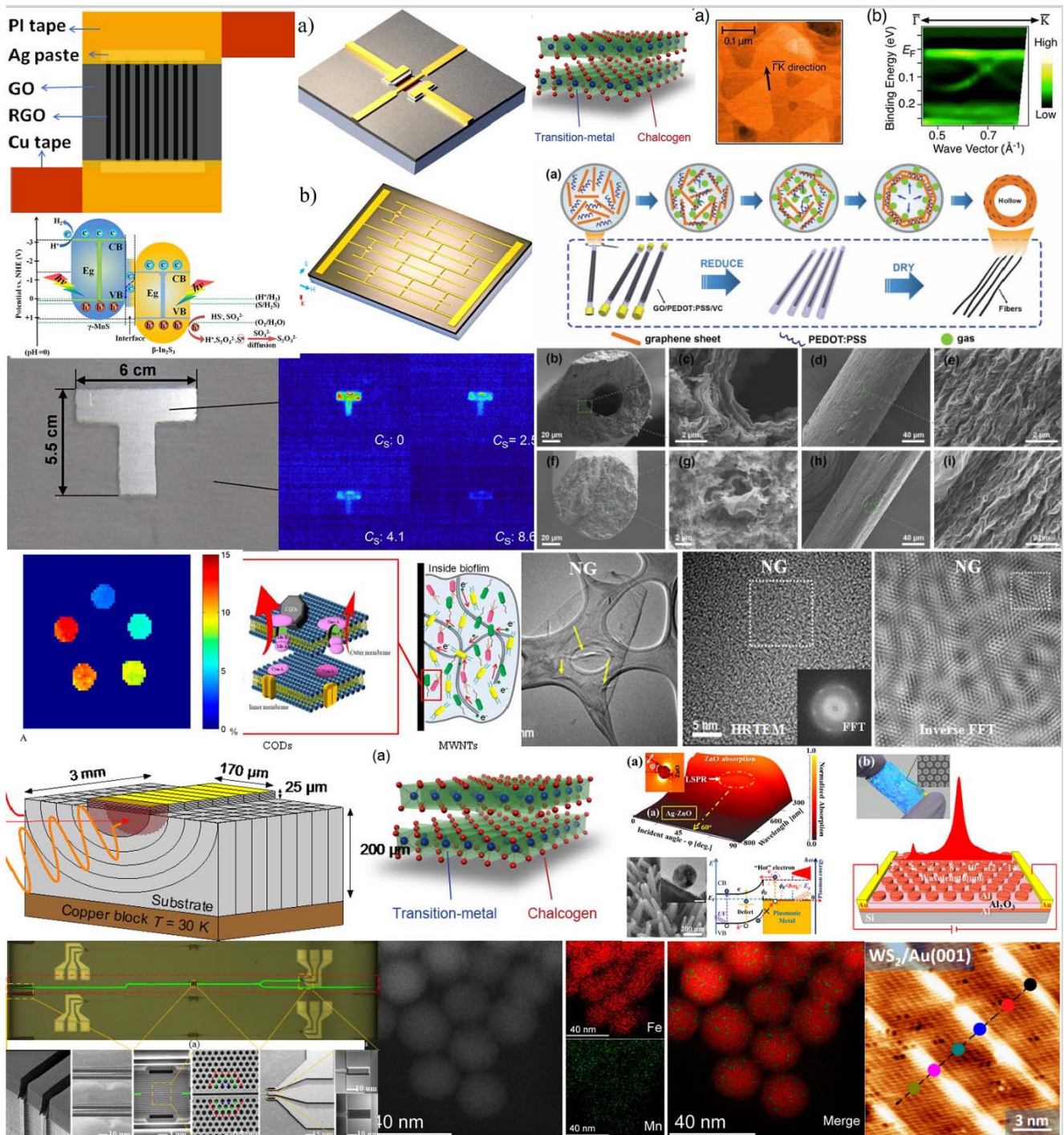


# Nano-Micro Conference 2017

# Conference Program

June 19-23, 2017, Shanghai, China



# Nano-Micro Conference 2017

June 19- 23, 2017 Shanghai, China



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## **General Information**

**Nano-Micro Conference 2017** is an international conference focused on Nano-Micro Science and Engineering. The aim of this conference is to bring together world-renowned experts, academicians, senior scientists, industry executives and project leaders from all over the world to discuss new developments and frontier researches in the multidisciplinary field of Nano-Micro Science and Engineering.

## **Conference Chair**

**Yafei Zhang**, Shanghai Jiao Tong University, China

## **Workshop Chairs**

**Weimin Chen**, Linköping University, Sweden

**Yujie Feng**, Harbin Institute of Technology, China

**Genquan Han**, Xidian University, China

**Kazuo Kadowaki**, University of Tsukuba, Japan

**Chaoyang Li**, Kochi University of Technology, Japan

**Guang Li**, Donghua University, China

**Hongjun Liu**, Xi'an Institute of Optics and Precision Mechanics, CAS, China

**Ho Seok Park**, Sungkyunkwan University, Korea

**Qiquan Qiao**, South Dakota State University, USA

**Liqiang Mai**, Wuhan University of Technology, China

**Donald K. Roper**, University of Arkansas, USA

**Yumeng Shi**, Shenzhen University, China

**Kimiyasu Shiraki**, University of Toyama, Japan

**Kang L. Wang**, University of California Los Angeles, USA

**Zhenhai Xia**, University of North Texas, USA

**Zhangxiong Wu**, Soochow University, China

**Yaxin Zhang**, University of Electronic Science and Technology of China, China

**Jim P. Zheng**, Florida State University, USA

## **Advisory Committee Chair**

**Kang L. Wang**, University of California Los Angeles, USA

## **Scientific Program Committee Chair**

**Zhi Yang**, Shanghai Jiao Tong University, China

## **Organizing Committee Chair**

**Mingwang Fu**, The Hong Kong Polytechnic University Hong Kong SAR

## Session Chairs

**Teng Ben**, Jilin University, China

**Toshiaki Hattori**, University of Tsukuba, Japan

**Kazuo Kadowaki**, University of Tsukuba, Japan

**Atsushi Kanno**, National Institute of Information and Communications Technology, Japan

**Minoru Fujishima**, Hiroshima University, Japan

**Yanfeng Zhang**, Peking University, China

**Ho Seok Park**, Sungkyunkwan University, Korea

**Jyh-Chiang Jiang**, National Taiwan University of Science and Technology, Taiwan

**Zhenhai Xia**, University of North Texas, USA

**Xufeng Kou**, ShanghaiTech University, China

**Weimin Chen**, Linköping University, Sweden

**Yutaka Takaguchi**, Okayama University, Japan

**Chaoyang Li**, Kochi University of Technology, Japan

**Weining Wang**, Virginia Commonwealth University, USA

**Kimiyasu Shiraki**, University of Toyama, Japan

**Giuseppina Cerrato**, University of Torino, Italy

**Yi Dan**, Sichuan University, China

**Genquan Han**, Xidian University, China

**XiaoYu Peng**, Chongqing Institute of Green and Intelligent Technology, CAS, China

**Zhangxiong Wu**, Soochow University, China

**Yongchun Zhao**, Huazhong university of Science and Technology, China

**Heqing Tang**, South-Central University for Nationalities, China

**Renhua Wu**, Shantou University Medical College, China

**Qun Zhao**, The University of Georgia, USA

## Registration desk hours

The Nano-Micro Conference 2017 registration desk, located outside the meeting room, will be open during the following hours:

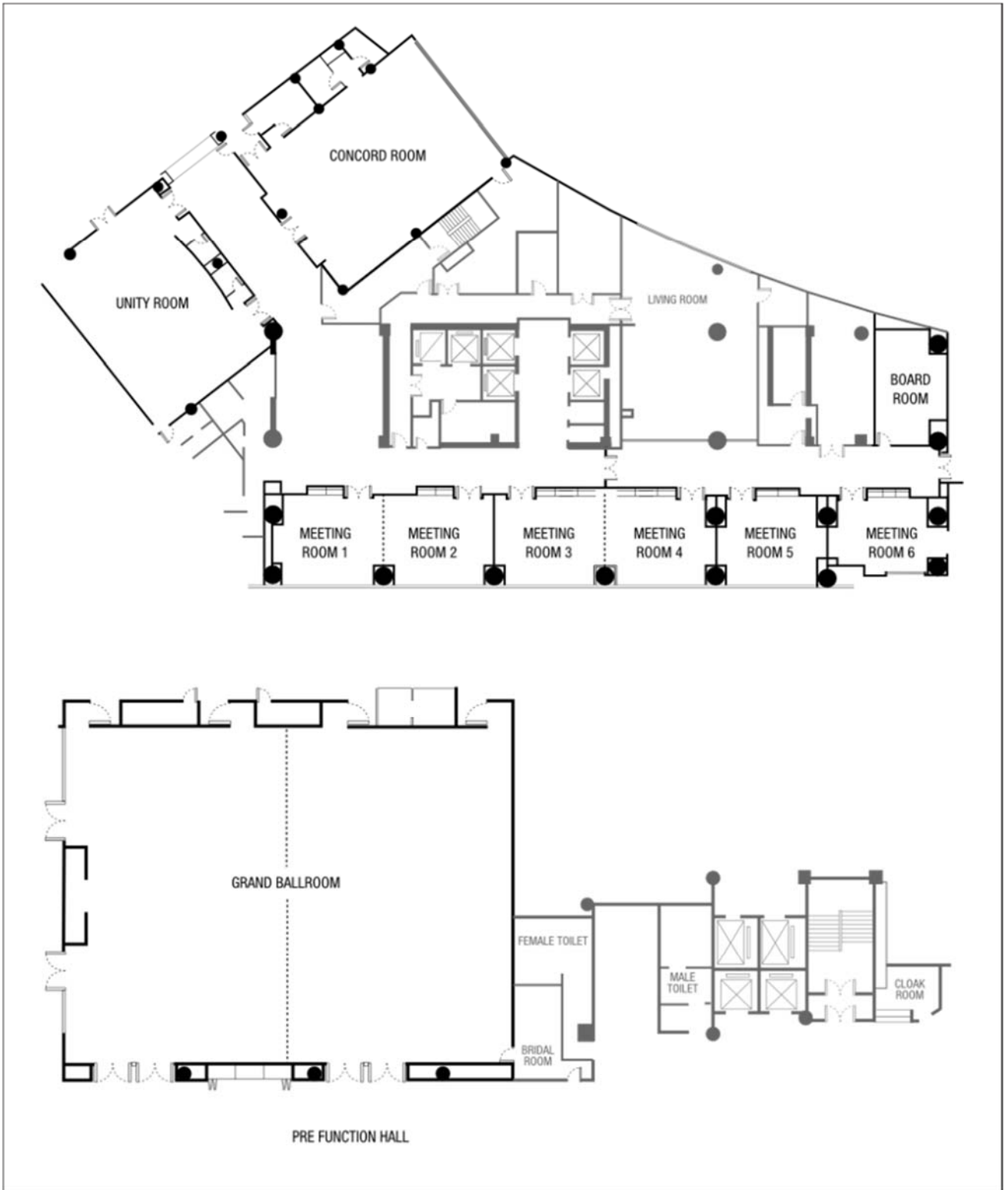
<b>Data</b>	<b>Time</b>
Monday, June 19th	2:00pm – 6:00pm
Tuesday, June 20 <sup>th</sup>	7:15am – 7:00pm
Wednesday, June 21 <sup>st</sup>	7:15am – 7:00pm
Thursday, June 22 <sup>nd</sup>	7:15am – 7:00pm

If you have questions, or need assistance, please don't hesitate to seek answer or help from the staffs in the registration desk.

# Conference Venue

**Location:** Shanghai Marriott Hotel Riverside, 99 Jiangbin Road, Shanghai 200023 China

**Meeting Room:** The third floor, MEETING ROOM 1(Room A), MEETING ROOM 2(Room B)





## Nano-Micro Conference 2017

June 19th – June 23rd

Shanghai Marriott Hotel Riverside, Shanghai, China

**Monday June 19**

14:00 – 18:00

Conference On-site Registration

Location: Shanghai Marriott Hotel Riverside

**Tuesday June 20**

**Room A**

**Session A1: Terahertz Technology**    **Chair: Toshiaki Hattori**

8:00-8:25AM	A01: Active imaging with incoherent sub-terahertz radiation in smoky environments	<b>Naofumi Shimizu</b> NTT Device Technology Labs, Japan
8:25-8:50AM	A02: Manipulate the terahertz waves using metallic gratings	<b>Renhao Fan</b> Nanjing University, China
8:50-9:10AM	A03: Modeling and Analysis of bow-tie antenna integrated resonant-tunneling-diode relaxation oscillators for wireless radio applications	<b>Hirokazu Yamakura</b> Tokyo Metropolitan University, Japan
9:10-9:35AM	A04: Coherent and Continuous Terahertz Emitters from High- $T_c$ Superconductor Mesa structures	<b>Kazuo Kadowaki</b> University of Tsukuba, Japan
9:35-10:00AM	A05: Transient Device Simulation Using Deterministic Boltzmann Equation Solvers	<b>Sung-Min Hong</b> Gwangju Institute of Science and Technology, Korea
10:00-10:20AM	Coffee Break	

**Session A2: Terahertz Technology**    **Chair: Kazuo Kadowaki**

10:20-10:45AM	A06: Terahertz semiconductor devices for photonic applications	<b>Hua Li</b> Shanghai Institute of Microsystem and Information Technology, CAS, China
10:45-11:10AM	A07: Making structured metals transparent for broadband electromagnetic waves	<b>Ruwen Peng</b> Nanjing University, China
11:10-11:35AM	A08: Terahertz-wave parametric wavelength conversion at room temperature	<b>Shin'ichiro Hayashi</b> National Institute of Information and Communications Technology, Japan

11:35-12:00PM	A09: Development of Small Size Terahertz Vacuum Sources in IECAS	<b>Wenxin Liu</b> Institute of Electronics, CAS, China
12:00-12:25PM	A10: Progressive in two-dimensional materials-based terahertz detection	<b>Lin Wang</b> Shanghai Institute of Technical Physics, CAS, China
12:00-14:00PM	Lunch Break	
<b>Session A3: Terahertz Technology    Chair: Atsushi Kanno</b>		
14:00-14:25PM	A11: 300GHz wireless link with a CMOS transceiver	<b>Minoru Fujishima</b> Hiroshima University, Japan
14:25-14:50PM	A12: Surface plasmon enhanced sub-Thz CMOS detector array	<b>Xiaoli Ji</b> Nanjing University, China
14:50-15:15PM	A13: Photonic crystal cavity optomechanics for the applications of low phase noise frequency source and high-performance sensing	<b>Yongjun Huang</b> University of Electronic Science and Technology of China, China
15:15-15:40PM	A14: Fast THz Modulator based on the stagger-netlike GaN HEMT active metamaterial	<b>Yaxin Zhang</b> University of Electronic Science and Technology of China, China
15:40-16:00PM	Coffee Break	
<b>Session A4: Terahertz Technology    Chair: Minoru Fujishima</b>		
16:00-16:25PM	A15: Hydration of various solutions observed by terahertz spectroscopy	<b>Toshiaki Hattori</b> University of Tsukuba, Japan
16:25-16:50PM	A16: Ultra-broadband Wireless Communications in the 0.1-10 Terahertz Band	<b>Chong Han</b> Shanghai Jiao Tong University, China
16:50-17:15PM	A17: Recent activities in the terahertz technology on communications and imaging	<b>Atsushi Kanno</b> National Institute of Information and Communications Technology, Japan
17:15-17:40PM	A18: Fundamentals of Terahertz Communication in Nanonetworks	<b>Xin-Wei Yao</b> Zhejiang University of Technology, China
17:40-18:05PM	A19: THz waveguide filters based on the periodic structures	<b>Ya-Xian Fan</b> Harbin Engineering University, China
19:00-22:00PM	<b>Conference Banquet</b>	

<b>Tuesday June 20</b>		
<b>Room B</b>		
<b>Session B1: Synthesis and Application of Transition-metal dichalcogenides</b>		
<b>Chair: Yanfeng Zhang</b>		
8:00-8:25AM	B01: Epitaxial Growth of Two-Dimensional Layered Transition-Metal Dichalcogenides and Heterostructures for 2D-Electronics	<b>Yumeng Shi</b> Shenzhen University, China
8:25-8:50AM	B02: Hysteresis of Transfer Characteristics in Field-Effect Transistors with a Molybdenum Disulfide Channel	<b>Yoshihiro Shimazu</b> Yokohama National University, Japan
8:50-9:15AM	B03: Valley Edelstein Effect in Monolayer Transition Metal Dichalcogenides	<b>Katsuhisa Taguchi</b> Nagoya University, Japan
9:15-9:40AM	B04: Growth of TMDC Nanostructures by Chemical Vapor Deposition	<b>Toshihiro Shimada</b> Hokkaido University, Japan
9:40-10:05AM	B05: Electrocatalytic hydrogen evolution reaction of MX <sub>2</sub> and MX <sub>2</sub> heterostructures	<b>Yanfeng Zhang</b> Peking University, China
10:05-10:20AM	Coffee Break	
<b>Session B2: Silicon for Energy Storage</b>		
<b>Chair: Ho Seok Park</b>		
10:20-10:45AM	B06: Pre-lithiated Si nanoparticles-carbon nanotubes composite anodes for Li-ion batteries	<b>Jim P. Zheng</b> Florida State University, USA
10:45-11:10AM	B07: Investigating structure and stress evolution in Si anode using in situ high pressure technique and Raman microscopy	<b>Zhidan Zeng</b> Center for High Pressure Science & Technology Advanced Research, China
11:10-11:35AM	B08: Silicon-based anode materials for high capacity lithium ion batteries	<b>Chuanbo Li</b> Institute of Semiconductors, CAS, China
11:35-12:00PM	B09: Efficient Solar-Rechargeable Lithium Ion Battery Energy Storage	<b>Qiquan Qiao</b> South Dakota State University, USA
12:00-14:00PM	Lunch Break	



<b>Session B3: Nanotechnology for Solar Energy Collection and Conversion</b> <b>Chair: Jyh-Chiang Jiang</b>		
14:00-14:25PM	B10: High performances flexible energy storage devices	<b>Bin Wang</b> Institute of Chemical Materials, CAS, China
14:25-14:50PM	B11: Porous carbon fibers for electromegnetic wave absorption	<b>Guang Li</b> Donghua University, China
14:50-15:15PM	B12: High Temperature Flexible Supercapacitors Using Graphene Electrodes	<b>Ho Seok Park</b> Sungkyunkwan University, Korea
15:15-15:40PM	B13: Rational design of Novel Carbon Catalysts for Clean Energy Conversion and Storage	<b>Zhenhai Xia</b> University of North Texas, USA
15:40-16:00PM	Coffee Break	
<b>Session B4: Graphene for Energy Storage</b> <b>Chair: Zhenhai Xia</b>		
16:00-16:25PM	B14: Kilohertz supercapacitors based on graphene and carbon fiber for AC filtering and energy harvesting	<b>Zhaoyang Fan</b> Texas Tech University, USA
16:25-16:50PM	B33: Composite AgBr colloidal spheres/g-C <sub>3</sub> N <sub>4</sub> nanosheets: An effective LED-irradiation photocatalyst	<b>Guochang Chen</b> Anhui University of Technology, China
16:50-17:15PM	B16: Laser direct writing of high-performance micro-supercapacitors on graphene oxide and polymer films	<b>Jinguang Cai</b> Institute of Materials, China Academy of Engineering Physics, China
17:15-17:40PM	B17: A First Principles study on doped Graphene decorated by metals for Enhanced Hydrogen Storage Performance	<b>Jyh-Chiang Jiang</b> National Taiwan University of Science and Technology, Taiwan
19:00-22:00PM	Conference Banquet	

<b>Wednesday June 21</b>		
<b>Room A</b>		
<b>Session A5: Topological Insulator Chair: Xufeng Kou</b>		
8:00-8:25AM	A20: Spin texture of flatten Dirac-cone surface state on W(110)	<b>Koji Miyamoto</b> Hiroshima University, Japan
8:25-8:45AM	A21: Chiral modes of topological semimetals under magnetic field	<b>Xiao-Xiao Zhang</b> The University of Tokyo, Japan
8:45-9:10AM	A22: Spin texture and spin injection in a 3D topological insulator	<b>Weimin Chen</b> Linköping University, Sweden
9:10-9:35AM	A23: Two dimensional topological insulators: progress and prospects	<b>Liangzhi Kou</b> Queensland University of Technology, Australia
9:35-10:00AM	A24: Charge-current induced spin polarization in BiSbTeSe <sub>2</sub> topological insulators	<b>Fan Yang</b> University of Cologne, Germany
10:00-10:20AM	Coffee Break	
<b>Session A6: Topological Insulator Chair: Weimin Chen</b>		
10:20-10:45AM	A25: Novel Topological Phase with a Zero Berry Curvature	<b>Feng Liu</b> Kwansei Gakuin University, Japan
10:45-11:10AM	A26: 2D materials-assisted fiber device as a novel nonlinear optical platform for multiwavelength ultrafast photonics	<b>Bo Guo</b> Harbin Engineering University, China
11:10-11:35AM	A27: Quantum phase transitions and order parameters of a topological insulator	<b>Yanchao Li</b> University of Chinese Academy of Sciences, China
11:35-12:00PM	A28: One-dimensional edge states with spin splitting in bismuth	<b>Akari Takayama</b> University of Tokyo, Japan
12:00-12:25PM	A29: Magnetic Topological Insulators and Their Heterostructures	<b>Xufeng Kou</b> ShanghaiTech University, China
12:25-14:00PM	Lunch Break	

<b>Session A7: Nanotechnology for Solar Energy Collection and Conversion</b> <b>Chair: Yutaka Takaguchi</b>		
14:00-14:25PM	A30: Green semiconductor vertical-cavity surface-emitting lasers based on quantum dots	<b>Bao-Ping Zhang</b> Xiamen University, China
14:25-14:50PM	A31: Titanium Dioxide Films with Pure Anatase Phase Synthesized by Mist Chemical Vapour Deposition	<b>Chaoyang Li</b> Kochi University of Technology, Japan
14:50-15:15PM	A32: Tuning solar absorbance and reflection of high-temperature solar spectrally selective surfaces	<b>Feng Cao</b> Harbin Institute of Technology Shenzhen Graduate School, China
15:15-15:40PM	A33: Broadband Optical Absorption Based on Plasmonic Nanostructures	<b>Qiang Li</b> Zhejiang University, China
15:40-16:00PM	Coffee Break	
<b>Session A8: General Chair: Chaoyang Li</b>		
16:00-16:25PM	A34: Unsteady flow and heat transfer of MHD nano-liquid thin film over a stretching sheet under thermocapillarity effect	<b>Yan Zhang</b> Beijing University of Civil Engineering and Architecture, China
16:25-16:50PM	A35: Focusing and Separating Diamagnetic Microparticles with Multiphase Ferrofluids	<b>Cheng Wang</b> Missouri University of Science and Technology, USA
16:50-17:15PM	A36: Semiconductor materials with open nanostructures for solar light-driven water splitting	<b>Changlong Chen</b> Jinan University, China
17:15-17:40PM	A37: H <sub>2</sub> -evolving SWCNT Photocatalysts for Effective Use of Solar Energy	<b>Yutaka Takaguchi</b> Okayama University, Japan
17:40-18:05PM	A38: One-Dimensional Nanomaterials for Energy Storage	<b>Liqiang Mai</b> Wuhan University of Technology, China
18:30-22:00PM	<b>Get-together Dinner</b>	

<b>Wednesday June 21 Room B</b>		
<b>Session B5: Nanostructured Photocatalysts and Their Applications Chair: Weining Wang</b>		
8:00-8:25AM	B19: Photocatalytic elimination of organic chemicals and aerosol-associated influenza virus infectivity in the air	<b>Kimiyasu Shiraki</b> University of Toyama, Japan
8:25-8:50AM	B20: Highly effective ZnO based nanoparticles in organic dyes removal	<b>Swee-Yong Pung</b> University of Science, Malaysia
8:50-9:15AM	B21: Nanostructured TiO <sub>2</sub> with oxygen vacancies for the decomposition of organics	<b>Chiaki Terashima</b> Tokyo University of Science, Japan
9:15-9:40AM	B22: TiO <sub>2</sub> -C hybrid aerogel photocatalysts for methylene blue degradation	<b>Rui Zhang</b> Shanghai Institute of Technology, China
9:40-10:05AM	B23: Highly efficient visible-light-driven BiVO <sub>4</sub> -based semiconductor photocatalysts	<b>Qizhao Wang</b> Northwest Normal University, China
10:05-10:20AM	Coffee Break	
<b>Session B6: Nanostructured Photocatalysts and Their Applications Chair: Kimiyasu Shiraki</b>		
10:20-10:45AM	B24: Highly Concentrated CO Evolution for Photocatalytic Conversion of CO <sub>2</sub> by H <sub>2</sub> O as an Electron Donor	<b>Kentaro Teramura</b> Kyoto Univerisity, Japan
10:45-11:10AM	B25: Nanostructured photocatalysts for the photocatalytic reduction of CO <sub>2</sub>	<b>Yunxiang Pan</b> Hefei University of Technology, China
11:10-11:35AM	B26: New Heterogeneous Photocatalysts Designed for Water Oxidation and CO <sub>2</sub> Reduction	<b>Kazuhiko Maeda</b> Tokyo Institute of Technology, Japan
11:35-12:00PM	B27: Facile Development of Nanostructured Photocatalysts for CO <sub>2</sub> Capture and Conversion	<b>Weining Wang</b> Virginia Commonwealth University, USA
12:00-14:00PM	Lunch Break	

<b>Session B7: Nanostructured Photocatalysts and Their Applications</b> <b>Chair: Giuseppina Cerrato</b>		
14:00-14:25PM	B28: Low Dimensional Materials Used for Lithium / Sodium ion Battery Anode	<b>Meicheng Li</b> North China Electric Power University, China
14:25-14:50PM	B29: Noble-metal free Metal sulphides as highly efficient visible light driven photocatalysts for H <sub>2</sub> production from H <sub>2</sub> S	<b>Ying Zhou</b> Southwest Petroleum University, China
14:50-15:15PM	B30: Photoelectrocatalytic Production of Solar Fuels from Water and CO <sub>2</sub>	<b>Hyunwoong Park</b> Kyungpook National University, Korea
15:15-15:40PM	B31: Significant photocatalytic enhancement via strengthening interface with TiO <sub>2</sub> by carboxyl-functionalized conjugated polymers	<b>Yi Dan</b> Sichuan University, China
15:40-16:00PM	Coffee Break	
<b>Session B8: Nanostructured Photocatalysts and Their Applications</b> <b>Chair: Yi Dan</b>		
16:00-16:25PM	B32: Ag nano-doping onto microsized TiO <sub>2</sub> : a challenge for enhancing the photocatalytic abatement of air pollution under visible light	<b>Giuseppina Cerrato</b> University of Torino, Italy
16:25-16:50PM	B15: Functionalized graphene with both physical and chemical adsorptions of charges for high-performance supercapacitors	<b>Jinzhong Liu</b> Beihang University, China
16:50-17:15PM	B34: Enhanced Catalysis by Optical Nanoantenna Reduced on Transition Metal Dichalcogenide	<b>Donald K. Roper</b> University of Arkansas, USA
17:15-17:40PM	B35: Synergistic effect of MoS <sub>2</sub> /TiO <sub>2</sub> heterostructures with enhanced photo- and electro-catalytic performance	<b>Junguang Tao</b> Hebei University of Technology, China
18:30-22:00PM	Get-together Dinner	

<b>Thursday June 22</b>		
<b>Room A</b>		
<b>Session A9: Terahertz Technology    Chair: Genquan Han</b>		
8:00-8:25AM	A39: Terahertz filter and demultiplexer with photonic crystal waveguide	<b>Hongjun Liu</b> Xi'an Institute of Optics and Precision Mechanics, CAS, China
8:25-8:50AM	A40: THz radiation based on fiber-integrated photo-conductive antennas and mode-locked Yb-doped fiber laser	<b>Min Yong Jeon</b> Chungnam National University, Korea
8:50-9:15AM	A41: Generation and Detection of the Super Broadband Terahertz Radiation based on Laser-plasma Interaction	<b>XiaoYu Peng</b> Chongqing Institute of Green and Intelligent Technology, CAS, China
9:15-9:40AM	A42: The fascinating split-ring-resonators: progress in design, fabrication and applications of terahertz metamaterials	<b>Mei Zhu</b> Taishan University, China
9:40-10:05AM	A43: Broadband terahertz absorber based on sinusoidally-patterned graphene	<b>Longfang Ye</b> Xiamen University, China
10:05-10:20AM	Coffee Break	
<b>Session A10: Terahertz Technology    Chair: Xiaoyu Peng</b>		
10:20-10:45AM	A44: Engineering rainbow trapping and releasing in ultrathin THz plasmonic graded metallic grating strip with thermo-optic material	<b>Genquan Han</b> Xidian University, China
10:45-11:10AM	A45: Micro-fabricated L-shape metasurface terahertz biosensor	<b>Jun Zhou</b> University of Electronic Science and Technology of China, China
11:10-11:35AM	A46: Intensity and spectral changes in terahertz quantum cascade lasers induced by the injection of near-infrared optical pulses	<b>Yohei Sakasegawa</b> National Institute of Information and Communications Technology, Japan
11:35-12:00PM	A47: THz surface/Interface Emission spectroscopy and applications	<b>Xinlong Xu</b> Northwest University, China
12:00-14:00PM	Lunch Break	



<b>Session 11 Porous Carbon Materials Chair: Zhangxiong Wu</b>		
14:00-14:25PM	A48: Design and electrochemical performance of nano-micro structured porous materials	<b>Yingke Zhou</b> Wuhan University of Science and Technology, China
14:25-14:50PM	A49: Molecular Insights into Electrical Double Layers in Graphene-Based Supercapacitors	<b>Guang Feng</b> Huazhong university of Science and Technology, China
14:50-15:15PM	A50: Preparation of novel microporous organic frameworks	<b>Teng Ben</b> Jilin University, China
15:15-15:40PM	A51: Porous Carbons and Polymers for Gas Mixture	<b>Yunfeng Zhao</b> Tianjin University of Technology, China
15:40-16:00PM	Coffee Break	
<b>Session A12: General Chair: Teng Ben</b>		
16:00-16:25PM	A52: Controllable Synthesis of N-Doped and Dually Doped Mesoporous Carbons for Adsorption and Catalysis Applications	<b>Zhangxiong Wu</b> Soochow University, China
16:25-16:50PM	A53: Accelerating the extracellular electron transfer of <i>Shewanella oneidensis</i> MR-1 by decorating cytochromes with carbon quantum dots and MWNTs	<b>Yujie Feng</b> Harbin Institute of Technology, China
16:50-17:15PM	A54: Application of transition-metal dichalcogenides beyond general electronics	<b>Yijin Zhang</b> Max-Planck-Institute for Solid State Research, Germany
18:30-21:00PM	<b>Get-together Dinner</b>	

<b>Thursday June 22</b>		
<b>Room B</b>		
<b>Session B9: Nanostructured Photocatalysts and Their Applications</b>		
<b>Chair: Yongchun Zhao</b>		
8:00-8:25AM	B36: Nano Photocatalytic Materials Design Toward Small Molecular Hydrocarbons Oxidation	<b>Zhiguo Yi</b> Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, China
8:25-8:50AM	B37: Ternary Nanostructured Photocatalysts for Photoelectrochemical Water Splitting	<b>Meng Nan Chong</b> Monash University Malaysia, Malaysia
8:50-9:15AM	B38: Photocatalytic Degradation of Polybrominated Diphenyl Ethers on TiO <sub>2</sub> -based composites	<b>Heqing Tang</b> South-Central University for Nationalities, China
9:15-9:40AM	B39: One-dimensional nanoarrays for solar cells	<b>Hao Wang</b> Hubei University, China
9:40-10:05AM	B40: Full-spectrum photocatalysts with Near-infrared activity	<b>Wenxia Liu</b> Qilu University of Technology, China
10:05-10:20AM	Coffee Break	
<b>Session B10: Nanostructured Photocatalysts and Their Applications</b>		
<b>Chair: Heqing Tang</b>		
10:20-10:45AM	B41: Nanowire-plasmonic photocatalysts and thermal emitters	<b>Thang Duy Dao</b> National Institute for Materials Science, Japan
10:45-11:10AM	B42: Van der Waals Oxide Heteroepitaxy for Transparent and Flexible Electronics	<b>Ying-Hao Eddie Chu</b> National Chiao Tung University, Taiwan
11:10-11:35AM	B43: N-doped graphene as highly-catalytic counter electrode in Dye-sensitized Solar Cells (DSSCs)	<b>Peng Zhai</b> Northwestern Polytechnical University, China
11:35-12:00PM	B44: CO <sub>2</sub> photocatalytic reduction using TiO <sub>2</sub> nanocrystals with coexposed {001} and {101} facets	<b>Yongchun Zhao</b> Huazhong university of Science and Technology, China

12:00-14:00PM	Lunch Break	
<b>Session B11: Nanotechnology for Magnetic Resonance Imaging</b> Chair: Renhua Wu		
14:00-14:25PM	B45: Albumin-mediated Gold/Platinum Nanocomposites for Dual Mode CT/MR Imaging Applications	<b>Nengqin Jia</b> Shanghai Normal University, China
14:25-14:50PM	B46: Manganese oxide-embedded iron oxide nanoparticles: An enhanced T1-T2 dual-modal contrast agent	<b>Chichong Lu</b> Beijing Technology and Business University, China
14:50-15:15PM	B47: Tracking of stem cells with Magnetic Resonance Imaging	<b>Qun Zhao</b> The University of Georgia, USA
15:15-15:40PM	B48: Surface passivation of magnetic nanoparticles via atomic layer deposition	<b>Rong Chen</b> Huazhong university of Science and Technology, China
15:40-16:00PM	Coffee Break	
<b>Session B12: Nanotechnology for Magnetic Resonance Imaging</b> Chair: Qun Zhao		
16:00-16:25PM	B49: Proteins promote cancer nanotheranostics	<b>Bingbo Zhang</b> Tongji University, China
16:25-16:50PM	B50: Nanoparticles in Magnetic Resonance Imaging	<b>Renhua Wu</b> Shantou University Medical College, China
16:50-18:00PM	Poster Session	
18:45-21:00PM	Get-together Dinner	

Poster Session		
P1	Two color optical absorption in InAs/AlSb/GaSb quantum well	<b>Xiangfei Wei</b> West Anhui University, China
P2	Enhanced electrochemical energy storage of N-doped graphene by adsorbing molecules of hydrolyzed polyimide	<b>Yi Zhao</b> Beihang University, China
P3	Gram-scale production of nanoporous graphene by Mg-thermoreduction of CS <sub>2</sub> for electrochemical energy storage	<b>Lu Sun</b> Beihang University, China
P4	Novel Self-powered UV-Visible Photodetector with Fast Response and High Photosensitivity Employing Fe:TiO <sub>2</sub> /n-Si Heterojunction	<b>Lin Sun</b> Donghua University, China
P5	Quasi-Freestanding Monolayer Striped WS <sub>2</sub> with an Invariable Band Gap on Au(001)	<b>Min Hong</b> Peking University, China
P6	Continuous and high-efficient synthesis of graphene oxide based on modified hummers method	<b>Xiaoshan Zhang</b> Guangxi University, China
P7	TBD	<b>Tianjiao Huang</b> Guangxi University, China
P8	Recent research in the continuous terahertz wave on nondestructive detection of carbon fibre composite	<b>Tielin Lu</b> Instrumentation Technology & Economy Institute(ITEI), China

<b>Friday June 23</b>	
9:00-10:00AM	Award Winners Announcement
10:00-12:00PM	Shanghai Natural History Museum tourism
12:00-13:30PM	Lunch Break
13:30-17:00PM	Shanghai Excursion(Chinese Culture, City God Temple of Shanghai, Yu Garden)

\*Invited Speakers are listed in Time, Talk Title, Name, Affiliation and Country/Region

**Session A1**

**A01**

**8:00 - 8:25 AM Room A June 20**

## Active imaging with incoherent sub-terahertz radiation in smoky environments

**NAOFUMI SHIMIZU**

NTT Device Technology Laboratories, NTT Corporation  
3-1 Morinosato-Wakamiya, Atsugi, Kanagawa, 243-0198 Japan  
Email: shimizu.naofumi@lab.ntt.co.jp

**KEN MATSUYAMA**

Center for Fire Science and Technology, Tokyo University of Science  
2641 Yamazaki, Noda, Chiba, 278-8510 Japan

### **Abstract**

This paper describes the capability of active imaging with sub-terahertz (THz) illumination in a smoky environment. The developed illuminator consists of nine uni-traveling-carrier photodiode modules and an optical circuit that generate incoherent sub-THz waves with a center frequency of 833 GHz. Tests on a target at a distance of 115 cm showed that imaging with incoherent sub-THz illumination provides a clear view in black, dense, and high-temperature smoke, for which the visibility was 30 cm for visible light. These results indicate that sub-THz active imaging is an effective way to ensure visibility in fire environments such as a space filled with heavy smoke.

### **Introduction**

Stringent building codes have improved fire protection and resistance. However, it is impossible to completely prevent outbreaks of fire in buildings. This is mainly because of careless human activities and appliance/equipment malfunctions and because it is very difficult for us to live without flammable daily commodities such as paper, fabrics, and plastics. Therefore, we must always on guard against outbreaks of fires.

One of the dangerous elements at the scene of a fire is smoke. Smoke is a mixture of air, airborne particles, and gases emitted during combustion or pyrolysis. Most of the particles range in size from 0.1 to 1  $\mu\text{m}$  [1]. Since the size is comparable to the wavelength of light, smoke particles strongly scatter light. As a result, dense smoke can reduce the visibility to zero. The lack of visibility makes it difficult for people to evacuate safely not only from unfamiliar places but also from familiar ones. It also obstructs the activities of even well-trained fire fighters with complete equipment.

Terahertz (THz) waves have a much longer wavelength than the diameter of smoke particles and can penetrate smoke [2-5]. If they can be used to observations, a clear view can be ensured even in severe smoky environments with poor visibility. THz imaging can be done actively or passively, and both methods are currently under intensive study. However, active THz imaging, which uses a high-brightness THz illuminator, is much better for observing objects in smoke. This is because smoke that has been heated to high temperature by fire becomes a strong source of thermal radiation—one that is

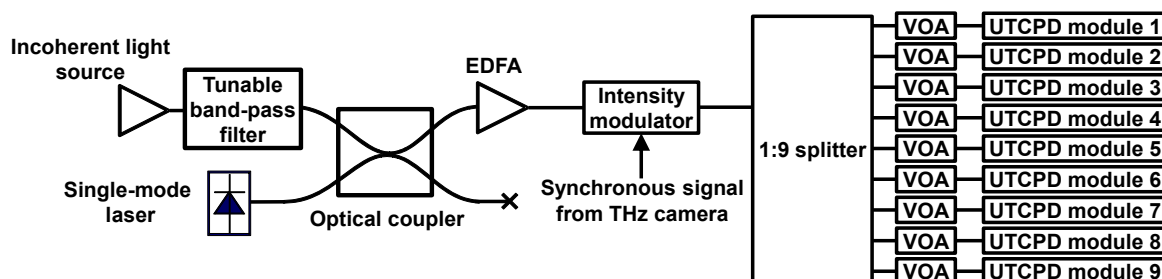


much stronger than the thermal radiation from the targeted room-temperature objects and completely masks them. The masking makes it impossible to detect objects by passive methods.

Taking the need for fire safety and the transmission and radiation characteristics of electromagnetic waves in smoke into consideration, we carried out feasibility studies on active imaging with sub-THz waves in smoky environments and produced certain results that demonstrated its effectiveness in ensuring a clear view in smoke [6-8]. In this paper, we present the experimental results obtained in an environment that simulates fires most faithfully among those studies.

### Sub-THz illuminator

The primary source of the sub-THz waves used as illumination was a broadband noise signal in the sub-THz region generated by a photomixer [9]. The signal's low coherency enables the simultaneous use of multiple photomixers to increase the brightness of the illumination. Figure 1 shows the optical circuit of the sub-THz illuminator, which consists of an incoherent light source, a tunable bandpass filter (BPF) with pass band width of 13 GHz, a single-mode laser, an optical coupler, and an erbium-doped fiber amplifier (EDFA), an intensity modulator, a 1:9 optical splitter, nine variable optical attenuators (VOAs), and nine uni-traveling-carrier photodiode (UTC-PD) modules with an integrated antenna [7, 10]. The BPF was used to tune the center frequency of the incoherent light, which was then coupled to the light from the single-mode laser. The resultant light was amplified by the EDFA and fed into the intensity modulator for on-off modulation. Finally, the signal was split into nine channels, each of which was sent through a VOA to a UTC-PD module. The center frequency of the incoherent sub-THz waves was 833 GHz, which falls within one of four frequency bands between 500 and 1000 GHz suitable for imaging in a space filled with smoke, gases, and other combustion products [6].



*Fig. 1. Schematic diagram of the optical circuit for generating incoherent sub-THz waves.*

Figure 2 shows the front view of the sub-THz illuminator [11]. Nine plano-convex lenses are attached to a 16-cm-diameter white polyethylene disk. One UTC-PD module is positioned behind each lens. A DC bias is applied to each module in parallel. The axes of the sub-THz beam emitted from the surrounding eight modules incline two degrees to the central beam axis. Therefore, the nine beam axes cross at approximately one meter in front of the disk. The power of the incoherent sub-THz waves emitted from the illuminator was estimated to be 5  $\mu$ W.



Fig. 2. Photograph of the sub-THz illuminator.

### THz camera and setup for imaging experiment

The imaging experiments employed a THz camera (Model T0832, NEC Corp.) equipped with a 2-inch-diameter aspherical plano-convex Tsurupica lens and a low-pass filter (LPF) [7]. The focal length of the lens and the cutoff frequency of the LPF are 36 mm and 1 THz. The THz camera was operated in the lock-in mode at a rate of 30 frames per second. A synchronous signal produced by the camera was sent to the intensity modulator of the optical circuit shown in Fig. 1. As a result, the intensity of the sub-THz waves from the illuminator was on-off modulated in synchronization with half of the frame rate of the camera. The camera continuously captured images with and without sub-THz illumination in an alternating sequence. The output image of the THz camera was a differential image between the illuminated image and the non-illuminated image. This process suppressed background noise in the output image.

For the imaging capability test in a smoky environment, a box-shaped structure consisting of an upper and a lower compartment with inside dimensions of 170 cm  $\times$  90 cm  $\times$  120 cm (LWH) was prepared [7]. The two compartments were separated by metal mesh, and the upper one contained a window on one of two walls facing the longitudinal direction. In the lower compartment, the incomplete combustion of thin latex film produced black smoke that filled the whole structure. A heating device that uses charcoal fire was also set in the lower compartment to raise the temperature of the smoke. A thermocouple attached to the wall of the structure measured the temperature of the smoke. During the experiment, the window was sealed with clear polyvinyl chloride film to keep the smoke inside the structure. The extinction coefficient of visible light,  $C_s$ , is a typical measure of the smoke density [1]. In this study, the intensity of the light emitted from an incandescent lamp set in the structure was monitored from the outside the window, and  $C_s$  in the structure was calculated [8].

The sub-THz illuminator and THz camera were placed 20 cm apart facing the window in the upper compartment at a distance of 20 cm from it. The target consisted of the letter T made of an aluminum plate and ceramic fiber board. Its width and height were 6 and 5.5 cm, respectively, as shown in Fig. 3. It was placed inside the upper compartment at a distance of 95 cm from the window. Thus, the distance from the illuminator to the target and the distance from the target to the camera were both 115 cm. The part of the aluminum plate exposed to the illuminator reflects back the irradiated sub-THz waves at a reflectance of nearly 100%. Therefore, an image of the T can be captured by the THz camera if a clear view to the target is achieved.

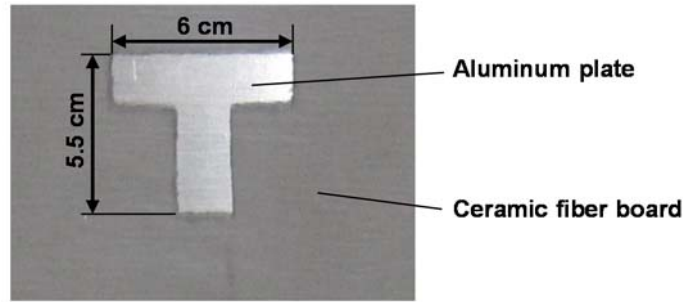


Fig. 3. Imaging test target.

### Results and discussion

Figure 4 shows  $C_s$  and the smoke temperature in the structure. Here,  $t = 0$  s is when the smoke source and the heating device were set on fire. Both  $C_s$  and the smoke temperature rose over time. Since maximum  $C_s$  of more than  $8 \text{ m}^{-1}$  and smoke temperature near  $150 \text{ }^\circ\text{C}$  were realized, a fire environment, such as a space filled with black, dense, and high-temperature smoke, was faithfully simulated in the structure.

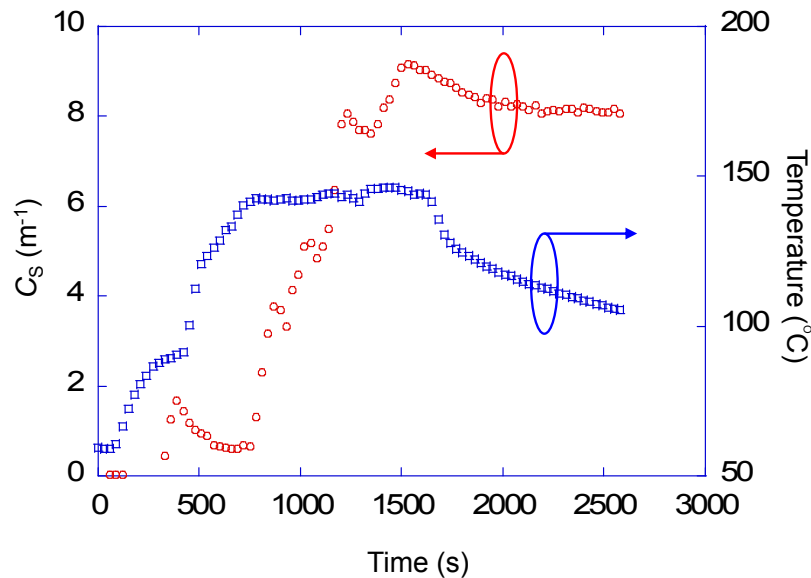


Fig. 4.  $C_s$  and smoke temperature inside the structure.

Figure 5 shows the images taken at  $t = 0, 360, 1020,$  and  $1230$  s. As shown in the images, the sub-THz imaging constantly provides a clear view of the target. Furthermore, the signal-to-noise ratio of the sub-THz image scarcely changes with  $C_s$  and smoke temperature. A  $C_s$  of  $8 \text{ m}^{-1}$  means a visibility of 30 cm for visible light [12]. Near-infrared light imaging done under the illumination by near-infrared light almost completely lost the view of the target at  $C_s$  of  $4.1 \text{ m}^{-1}$  in the control experiment, as shown in Fig. 6. These results indicate that sub-THz active imaging is an effective way to ensure visibility in fire environments such as a space filled with black, dense, and high-temperature smoke.

In this study, the distance between the target and camera was only around one meter. This distance limit will be improved to a level suitable for practical imaging in smoky environments when an advanced illuminator and THz camera are developed.

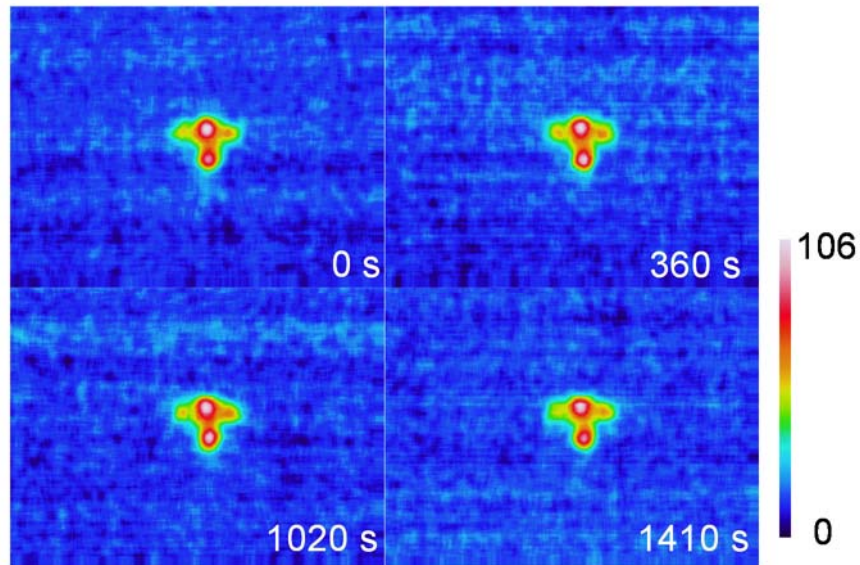


Fig. 5. Sub-THz image of target at  $t = 0, 360, 1020,$  and  $1410$  s.

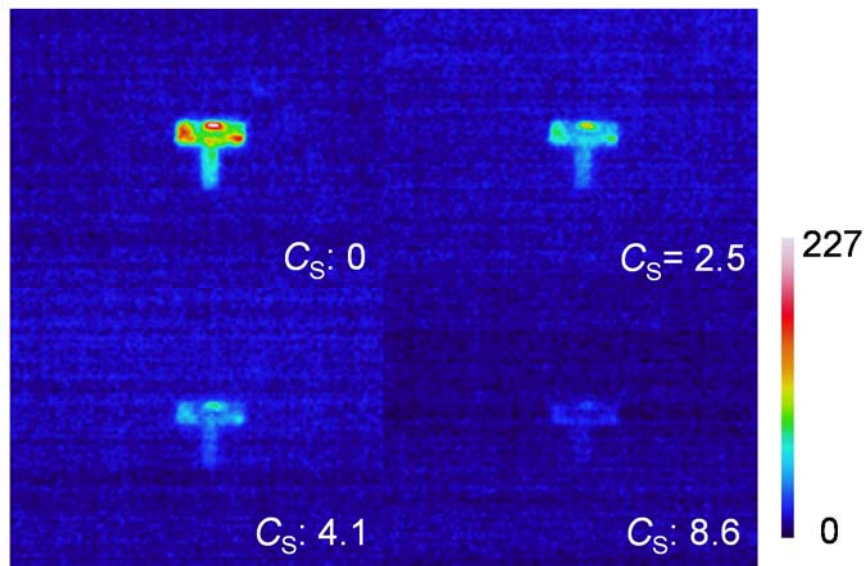


Fig. 6. Near infrared image of target at  $C_s = 0.0, 2.5, 4.1,$  and  $8.6$   $m^{-1}$ .

### Conclusion

The capability of active imaging with sub-THz illumination in a smoky environment was investigated. The source of the illumination was incoherent sub-THz waves generated by photomixing. Imaging tests performed under a condition that faithfully simulated a fire site showed that sub-THz active imaging provides a clear view in the space filled with black, dense, and high-temperature smoke with a visibility of 30 cm. The result indicates that active imaging with incoherent sub-terahertz radiation is an effective way to see through smoke at the scene of a fire.

### Acknowledgment

This work was supported in part by the Japan Science and Technology Agency.

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**Naofumi Shimizu** is Senior Research Engineer of NTT Device Technology Laboratories, Nippon Telegraph and Telephone Corporation. He is also a visiting professor of Center for Fire Science and Technology, Tokyo University of Science from 2016. He is a Member of IEEE, the Institute of Electronics, Information and Communication Engineers (IEICE), Japan, the Japan Society of Applied Physics, and the Japan Association for Fire Science and Engineering. He was a recipient of the 2002 IEICE Electronics Society Prize and the Best Paper Award of the 2006 Asia–Pacific Microwave Photonics Conference.



His current research interests include terahertz spectroscopic and imaging systems.



**Session A1**

**A02**

**8:25 - 8:50 AM Room A June 20**

## Tune the polarization of terahertz waves via subwavelength metallic gratings

REN-HAO FAN, RU-WEN PENG, AND MU WANG

National Laboratory of Solid State Microstructures, School of Physics, and Collaborative Innovation Center of Advanced Microstructures, Nanjing University  
Nanjing 210093, China  
Email: rhfan@nju.edu.cn

### Abstract

Here we present our recent work on tuning the polarization of terahertz waves via subwavelength metallic gratings. Firstly, we have experimentally demonstrated a linear polarization rotator that is a three-layer metallic grating structure for manipulating the polarization of broadband terahertz waves. By mechanical rotations of the composite grating layers, this freely tunable device can rotate the polarization of a linearly polarized THz wave to any desired direction with high conversion efficiency [1]. Then we theoretically investigate the propagation of terahertz waves through a graphene-loaded metal grating under external magnetic field. It is found that resonant modes in the system can be converted between transverse-electric and transverse-magnetic polarizations due to Hall conductivity of graphene, as a consequence, asymmetric transmission of terahertz waves through this graphene-loaded metal grating is achieved, and it can be tuned by adjusting either the external magnetic field or the Fermi level of graphene [2]. These tunable terahertz devices have potential applications in various areas, such as material analysis, wireless communication, and terahertz imaging.

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**Ren-Hao Fan** is Associate Professor of Physics, Nanjing University. His current research interests include Terahertz metamaterials, Terahertz spectroscopy, and Plasmonics.



*Session A1*

*A03*

*8:50 - 9:10 AM Room A June 20*

## Modeling and Analysis of Bow-Tie Antenna Integrated Resonant-Tunneling-Diode Relaxation Oscillators for Wireless Radio Applications

HIROKAZU YAMAKURA, MICHIIHIKO SUHARA

Department of Electrical and Electronic Engineering, Tokyo Metropolitan University

1-1, Minami-Osawa, Hachioji, Tokyo, 192-0397 JAPAN

yamakura-hirokazu@ed.tmu.ac.jp, suhara@tmu.ac.jp

### **Abstract**

We propose a self-complementary bow-tie antenna-integrated resonant-tunneling-diode relaxation oscillator and investigate its oscillation/radiation characteristics. In the investigation, we establish a physics-based equivalent circuit model of the oscillator for taking the all physical phenomena related to the diode and the antenna into consideration simultaneously. In this paper, we report the equivalent circuit modeling and the large-signal oscillation/radiation analysis of the oscillator.

### **Introduction**

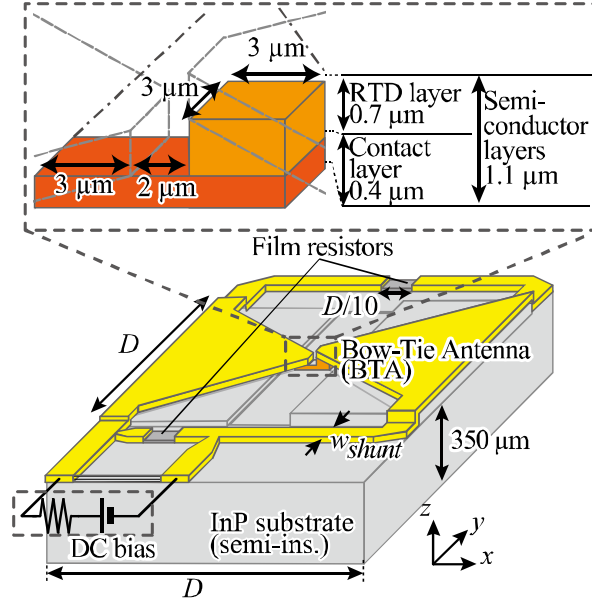
Terahertz (THz) technology has been received great deal of interest in terms of applications for spectroscopy, imaging, wireless communications, etc. In the wireless communication, the THz range is specifically one of the most attractive regions owing to the existence of the non-allocated frequency band. One of the main challenges of the THz wireless communication is the shortage of the emission RF power of the oscillator. We guess the challenge can be overcome by using the wideband-spectrum relaxation wave, whose entire emission RF power exceeds that of the narrowband sinusoidal wave, as the carrier.

From this perspective, we have proposed an oscillator consisting of a resonant tunneling diode (RTD) and a broadband bow-tie antenna (BTA) [1] for generating a wideband-spectrum relaxation wave and their theoretical models expressed by equivalent circuits respectively [2,3]. Such a semiconductor-based oscillator for THz applications is generally fabricated as a monolithically-integrated configuration of an oscillation device, a radiation antenna, etc. As the performance of such an oscillator depends upon a both of their physics, which usually differ from each other, the performance evaluation method and the design guideline for the oscillator should be established as a physical-coupled scheme considering the all effects regarding the oscillator simultaneously.

In this paper, we focus on a physics-based modeling for the entire oscillator-structure we proposed and its oscillation/radiation performance evaluated by using the physics-based model.

### **Modeling**

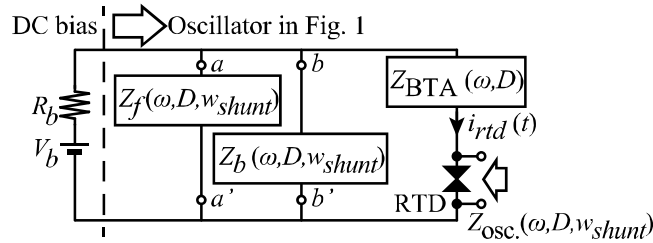
Schematics of the proposed oscillator are illustrated in Fig. 1.



**Fig.1** Schematics of a proposed oscillator

A peripheral circuit in front serves as a bias circuit and that in back is added for adjusting the total impedance of the peripheral circuits. We establish a physics-based equivalent circuit model of each component, RTD, BTA, and the circuits, since it is considerably impossible to analyze the quantum phenomena of the RTD together with the electromagnetic (EM) properties of the other components by a single solver.

Simple block expressions of the oscillator are described in Fig. 2.



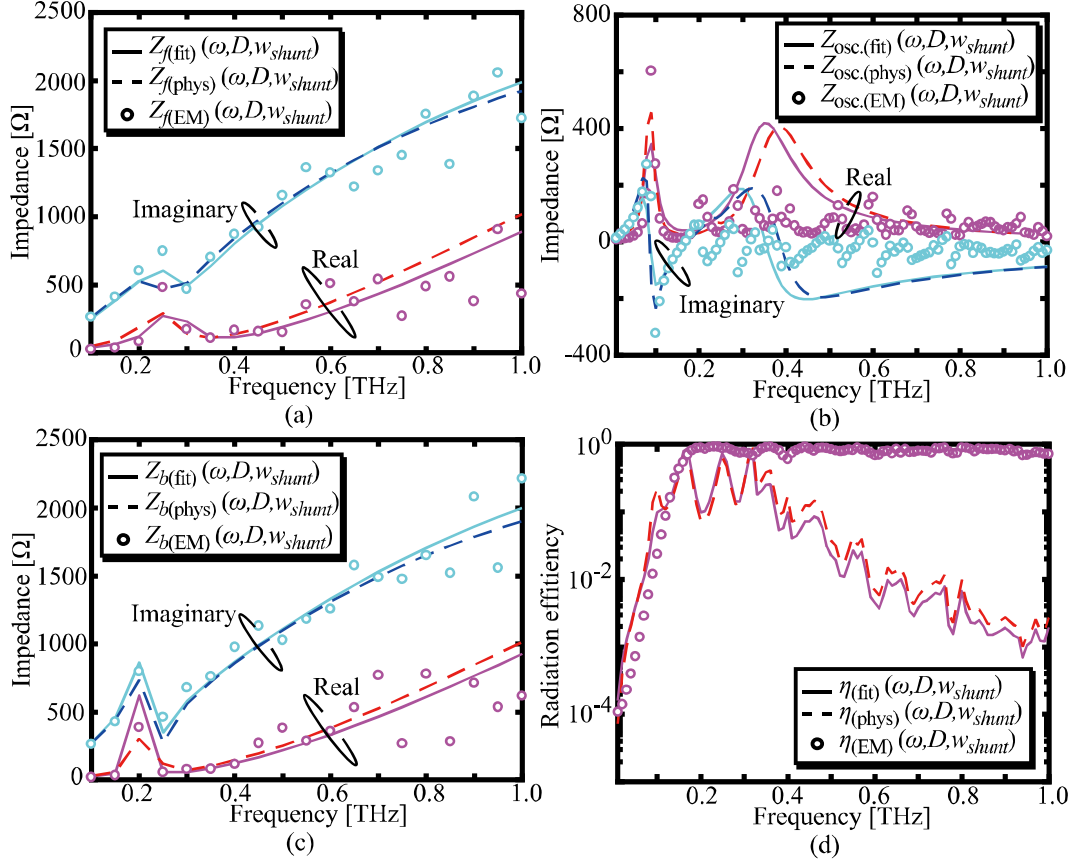
**Fig.2** Block expressions of an equivalent circuit for the oscillator shown in Fig. 1

The impedance variables,  $Z_f(\omega, D, w_{shunt})$ ,  $Z_b(\omega, D, w_{shunt})$ , and  $Z_{BTA}(\omega, D)$ , correspond to the equivalent circuit of the peripheral circuit in front, that in back, and the BTA, respectively. The RLC expression of  $Z_{BTA}(\omega, D)$  has been reported in Ref. [2]. Additionally, the circuit model of the RTD and its theoretical expression has also been reported in Refs. [3, 4], respectively.

The variables,  $Z_f(\omega, D, w_{shunt})$  and  $Z_b(\omega, D, w_{shunt})$ , are composed of several RLC elements which can be explained by the electromagnetic properties: the surface impedance due to the skin effect [5], the straight micro stripline [6], fringe capacitance [7], and parasitic components regarding the semi-insulating substrate. The circuit elements involved in  $Z_f(\omega, D, w_{shunt})$  and  $Z_b(\omega, D, w_{shunt})$  are evaluated by the EM field distribution in the vicinity of the circuits calculated by the finite element method-based simulator, namely, COMSOL. Their approximate numerical values of the elements are also estimated by the physical interpretation based on the structural and material properties. More precise values are numerically de-embedded by using the optimization method, namely, the particle swarm

optimization [8]. More details regarding the circuit identification process have also been reported in Ref. [2].

Figure 3 summarizes the typical fitting results of the impedance and radiation characteristics regarding the peripheral circuit/entire oscillator.



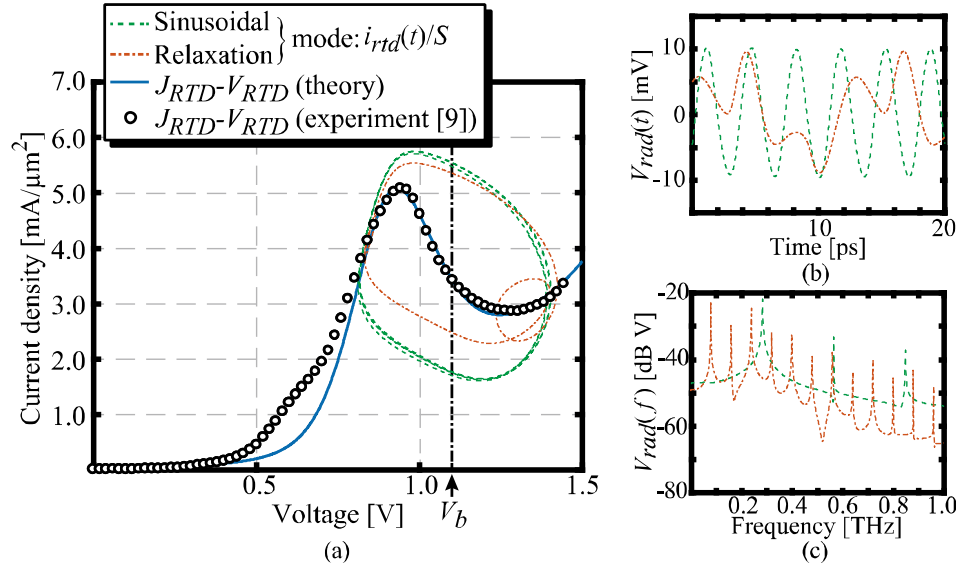
**Fig.3** Typical fitting results regarding the impedance characteristics of (a) the peripheral circuit in front, (b) that in back, and (c) the entire oscillator, and (d) the radiation characteristics. Radiation efficiency,  $\eta(\omega, D, w_{shunt})$ , is defined by the ratio of the oscillation power on the semiconductor layers to the radiation power on the BTA. Solid lines are depicted by using the de-embedded values of the circuit parameters. Dash lines are calculated by the physical/material parameters. The antenna size,  $D$ , and the line width,  $w_{shunt}$ , are set to 300 and 10  $\mu\text{m}$ , respectively.

From Fig. 3, the equivalent circuit expression is quantitatively valid for the evaluation of the radiation/oscillation characteristics by the circuit analysis around the first resonance frequency of the oscillator.

### Oscillation Analysis

The non-linear oscillation analysis of the proposed oscillator is performed by using the equivalent circuit above mentioned. The non-linearity of the RTD is involved by considering the measured current-voltage ( $I$ - $V$ ) characteristics [9]. The supplied voltage,  $V_b$ , is set to a constant value to keep the negative differential conductance of the RTD maximum. More details regarding the oscillation analysis methodology have been reported in Refs. [10, 11].

Figure 4 displays the current density-voltage ( $J$ - $V$ ) characteristics of the RTD and the time-dependent orbit of the current density,  $i_{rtd}(t)/S$ , in the RTD, where  $S$  indicates the mesa area.



**Fig.4** (a) Measured/theoretical current density-voltage ( $J$ - $V$ ) characteristics of the employed RTD and the calculated results of the time-dependent orbit of the current density,  $i_{rad}(t)/S$ , in the RTD. (b) Waveforms of the radiation voltage and (c) corresponding frequency spectra. Chain and dotted lines indicate the relaxation and the sinusoidal oscillation mode, where the line width,  $w_{shunt}$ , is set to 10 and 20  $\mu\text{m}$ , respectively. Antenna size,  $D$ , is set to 300  $\mu\text{m}$ .

We classify the oscillation modes depicted the dotted and chain lines in Fig. 4 designated as the "sinusoidal" and the "relaxation" mode, respectively. The modes are quantitatively distinguished by the cycle number of the  $i_{rad}(t)/S$  trajectory in Fig. 4; if the cycle number is unity, the mode is a "sinusoidal mode"; else, it is a "relaxation mode". The entire emission RF power of the relaxation mode shown in Fig. 4 is  $\sim 6$  dBm greater than that of the sinusoidal mode when the upper limit value of band is approximately set to 400 GHz. It is suggested that the relaxation wave can compensate for the shortage of the emission RF power if we employ a certain band appropriately. Moreover, it is found that the oscillation mode can be designed by adjusting the two parameters,  $D$  and  $w_{shunt}$ , appropriately.

According to Shannon-Hartley theorem [12], the capacity of a wireless channel is directly proportional to the channel bandwidth. Therefore, the wideband-spectrum relaxation wave can contribute to the possibility of large-capacity wireless transmissions together with compensating for the RF power shortage.

## Conclusion

We investigated radiation/oscillation characteristics of the resonant tunneling diode-based relaxation oscillator by using its physics-based equivalent circuit model. The advantage of a wideband-spectrum relaxation wave as the carrier was revealed in terms of the entire emission RF power. Our further studies will represent the link-budget analysis of the relaxation carrier wave-based THz wireless link to clarify the advantage of the relaxation carrier regarding the link performance.



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**Hirokazu Yamakura** is a Ph.D. candidate at Tokyo Metropolitan University, JAPAN. He received his B.S. and M.S. degrees in Electric and Electrical Engineering from Tokyo Metropolitan University in 2013 and 2015, respectively. He is a student member of the Institute of Electrical and Electronics Engineers (IEEE), the Institute of Electronics, Information and Communication Engineers (IEICE), and the Japan Society of Applied Physics (JSAP).



His current research interests include compound semiconductor terahertz devices and terahertz wireless communications.

**Session A1**

**A04**

**9:10 - 9:35 AM Room A June 20**

## Coherent and Continuous Terahertz Emitters from High- $T_c$ Superconductor Mesa structures

K. KADOWAKI<sup>1,2</sup>, T. YUASA<sup>1</sup>, T. TANAKA<sup>1</sup>, Y. KOMORI<sup>1</sup>, R. OTA<sup>1</sup>, G. KUWANO<sup>1</sup>, Y. TANABE<sup>1</sup>, K. NAKAMURA<sup>1</sup>, M. TSUJIMOTO<sup>1,2</sup>, H. MINAMI<sup>1,2</sup>, T. KASHIWAGI<sup>1,2</sup>

1. Graduate School of Pure & Applied Science, University of Tsukuba,  
1-1-1, Tennodai, Tsukuba, Ibaraki 205-8573, Japan,

2. Division of Materials Science, Faculty of Pure & Applied Sciences, University of Tsukuba,  
1-1-1, Tennodai, Tsukuba, Ibaraki 305-8573, Japan

Email: kadowaki@ims.tsukuba.ac.jp

RICHARD A. KLEMM

Department of Physics, University of Central Florida

Orlando, Florida 32816-2385, USA

Email: Richard.Klemm@ucf.edu

### Abstract

After the discovery of high temperature Superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  with the superconducting transition temperature  $T_c=92$  K, which is well above 77 K, the boiling point of liquid nitrogen, this year has become a celebrative and a commemorative 30<sup>th</sup> anniversary in the history of superconductivity research. In addition to this memorable occasion, this year is another important anniversary that ten years have passed after the discovery of terahertz electromagnetic wave emission from the mesa structure of Bi2212 single crystals[1]. The important ingredients here is that the superconducting  $\text{CuO}_2$  double layers are built in a unit cell of the Bi2212 crystal as it is grown and are sandwiched by the insulating  $\text{Bi}_2\text{O}_2$  layers, forming a stack of intrinsic Josephson junctions (IJJs). Since the electronic structure as a result of this layered crystal structure the superconducting as well as even normal state is highly two dimensional, the superconducting coupling becomes Josephson-junction like, extremely weak as measured by the c-axis critical current  $J_c^c = 10^2 - 10^3$  A/cm<sup>2</sup> compared with  $J_{ab}^c = 10^6 - 10^7$  A/cm<sup>2</sup>, resulting in the reduction of the superconducting plasma frequency to the level of  $f_J \sim 10^{11}$  c/s

(0.2 ~ 1 meV), which is well below the superconducting gap  $\Delta \sim 30$  meV. This Josephson plasma mode can be excited by the  $dc$ -current through the nonlinear Josephson coupling effect by the  $dc$ -Josephson effect and the coherent THz emission is generated due to the  $ac$ -Josephson oscillation with the frequency  $f_J = (2e/h)v_J$ , where  $e$  is the elementary charge of electron,  $h$  Planck constant, and  $v_J$  the voltage per intrinsic Josephson junctions, when it matches well the cavity mode frequency. Although the understanding of this phenomenon has already been well established by various experiments and theoretical works[2], the practical limitation of the device is not well understood yet. For example, the most important issue is on what determines the maximum power extracted from one intrinsic Josephson junction, and how much power can be generated from the actual mesa structure with  $N$ -intrinsic

Josephson junctions, where  $N$  is the number of intrinsic Josephson junctions in a mesa. The next issue is on what limits the maximum frequency.

The essential parameter related to two issues has evidently been thought the thermal effect due to the Joule heating by the dc-current (10 - 50 mW), which produces heat of  $\sim$ MW/cm<sup>3</sup> and naturally causes a serious temperature increase and inhomogeneity, which is often called as a hot-spot. It has been disclosed by us that the formation of the hot-spot gives only a detrimental effect on the THz radiation phenomena so that it is better to avoid it or control it to make the influence minimum on the THz emission. The heating issue has recently been studied intensively[3]. As a result, we have achieved a frequency of 2.4 THz with a power of 30  $\mu$ W[4] quite reproducibly.

Recently, we have done a systematic case study on the rectangular, square, circular, triangular mesas, *etc.* and found an interesting fact. That is concerning the missing modes, which are expected to be as the strong emission modes but systematically disappear or are missing, perhaps, due to very weak intensities. This seems to occur especially in the degenerated symmetric cases such as in square and circular mesas. We argue this effect as a mode cancellation in the degenerated cavity modes in a symmetric mesa.

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**Kazuo Kadowaki** is Professor of Institute of Materials Science University of Tsukuba. His research subjects are Low temperature solid state physics (superconductivity and magnetism). He got his Doctor degree of Science from Osaka University at 1980. From 1980 to 1981, he was a Research fellow at JSPS (Japan Society for the Promotion of Science) His research project was “High sensitivity magnetization measurements in low dimensional magnetic materials with SQUID magnetometer”. From 1981 to 1982, he was Yukawa Fellow and mainly studied on superconducting properties in superconductors with rare-earth ions. From 1982 to 1984, he was Postdoctoral Fellow, and then Research Associate in 1985, at Department of Physics, Alberta State University, Canada. His research project was “Single crystal growth and transport properties on heavy Fermion systems”. From 1986 to 1989, He was Researcher of Institute of Physics, and then Senior Researcher in 1989, at Amsterdam University. His research project was “Single crystal growth and physical properties on heavy Fermion systems and high-Tc superconductors”. From 1990 to 1993, he was Senior Researcher of National Research Institute for Metals, Japan. His research project was “Single crystal growth and physical properties on high-Tc superconductors”. From 1993 to 1995, he was Senior Researcher and Leader of 2nd Sub-group, 1st Research Group at National Research Institute for Metals, Japan. His research project was “Single crystal growth and physical properties on high-Tc superconductors and development of growth technique for high-purity and quality intermetallic single crystals”. From 1995 to 1997, he was Associate Professor of Institute of Materials Science, University of Tsukuba, Japan. His research project was “Single crystal growth and physical properties on high-Tc superconductors and high-purity intermetallic single crystals” From 1997 to present, he is Professor of Institute of Materials Science, University of Tsukuba, Japan. His research project is “Single crystal growth and physical properties on high-Tc superconductors and high-purity intermetallic single crystals”.



For more information, please visit:

[http://www.ims.tsukuba.ac.jp/~Kadowaki\\_lab/person/kadowaki/english/index.htm](http://www.ims.tsukuba.ac.jp/~Kadowaki_lab/person/kadowaki/english/index.htm).

*Session A1*

*A05*

*9:35 - 10:00 AM Room A June 20*

## Transient Device Simulation Using Deterministic Boltzmann Equations

### Solvers

SUNG-MIN HONG

Gwangju Institute of Science and Technology

123 Cheomdan-gwagiro (Oryong-dong), Buk-gu, Gwangju 61005, Republic of Korea

Email: smhong@gist.ac.kr

### Abstract

The transient simulation of semiconductor devices using a deterministic Boltzmann equations solver is presented. In order to avoid the numerical difficulties originated from the conventional  $H$ -transformation, the kinetic-energy-based scheme is adopted. Within the kinetic-energy-based scheme, the transport parameters become time-independent, therefore, implementing the transient simulation capability can be done easily. Preliminary results for a device are shown.

### Introduction

The terahertz (THz) technology has gained much research interest worldwide. However, realization of a THz emitter with a small form factor is still a difficult task. The plasma instability in the two-dimensional (2D) electron gas has been proposed as a possible mechanism to enable an extremely fast semiconductor device operating in the THz frequency range [1].

Recently, we have reported the numerical simulation results of plasma oscillation in two-dimensional electron gas [2]. A periodic steady-state solver has been used to obtain the oscillating solution efficiently. The set of governing equations contains the 2D Poisson equation, the electron continuity equation, and the electron current density equation. The time derivative of the current density and the convective derivative are considered in the electron current density equation. It has been numerically verified that inclusion of those terms are mandatory to support sufficiently strong plasma instability in the 2D electron gas.

However, it is noted that the set of governing equations adopted in [2] is based on the moments of the Boltzmann equation. It is not sufficiently accurate to describe the behaviour of plasma waves quantitatively [3]. A more advanced modelling approach is required. In order to solve this issue ultimately, the Boltzmann equation solver with the transient simulation capability is mandatory.

Although the stochastic Boltzmann equation solvers (the Monte Carlo simulators) have been used to simulate a device operating in the THz frequency range (for example, [4]), the stochastic nature of the Monte Carlo simulators introduces some numerical difficulties. Therefore, the deterministic Boltzmann equation solver is desirable. In this work, our motivation is to present some transient simulation results using a deterministic Boltzmann equation solver.

## Projected Boltzmann Equation

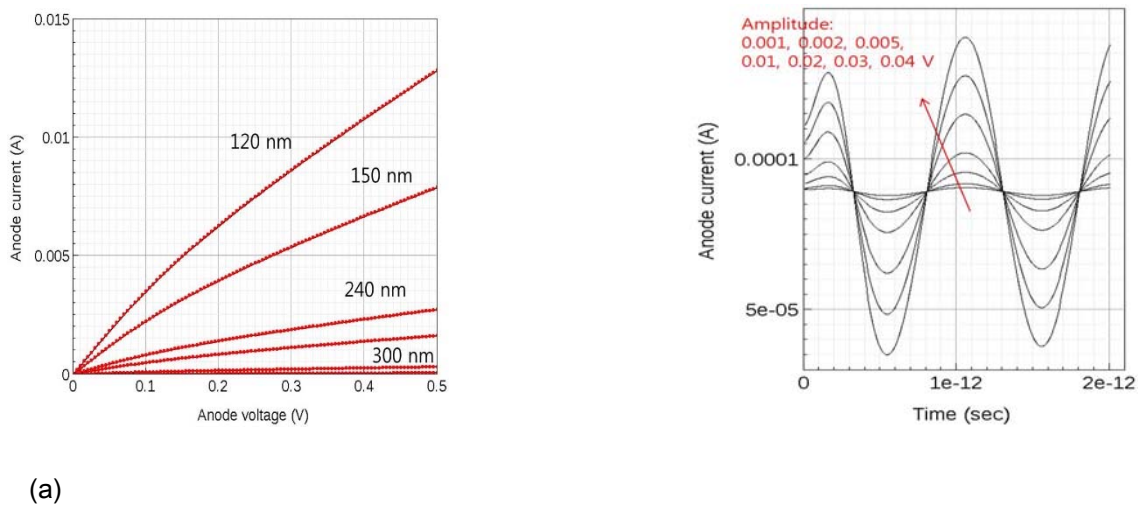
The Boltzmann equation is a microscopic transport equation. It governs the spatiotemporal motion of the electron gas in a semiconductor device. Since it is defined on the phase space, evaluating its solution is a highly non-trivial task.

As discussed above, the stochastic Monte Carlo method can be applied to solve the Boltzmann equation efficiently. However, nowadays, the deterministic Boltzmann equation solvers [5] have gained popularity. In these solvers, the angle-dependent part of the electron distribution function is expanded with basis functions. Depending on the dimensionality of the momentum space, there can be a few variants of deterministic Boltzmann equation solvers. In this work, the three-dimensional momentum space is understood. Therefore, the spherical harmonic expansion [6] is the appropriate technique. A numerical stabilization scheme called the  $H$ -transformation [6] has played an important role in the development of this simulation technique. In the  $H$ -transformation, the total energy (which is a sum of the kinetic energy and the potential energy) instead of the kinetic energy is used as the energy variable.

Unfortunately, when the transient simulation is concerned, the  $H$ -transformation introduces a serious difficulty [7]. The time-varying potential energy yields the time-varying transport parameters. Unavoidable interpolation procedure prevents the transient simulation capability eventually. Of course, the fundamental solution to the above problem is to invent yet another numerical stabilization scheme, which does not suffer from the time-varying transport parameters. Since it is currently a formidable task, in this work, we simply apply the kinetic-energy-based scheme [8] to get the preliminary solutions.

## Numerical Results

A spherical harmonics expansion solver has been newly implemented into our in-house device simulation framework [2]. All parameters for Si are taken from [6]. The lowest expansion order is used. Various  $N^+NN^+$  devices are simulated. Fig. 1(a) shows the DC IV characteristics of those devices. The transient simulation results of the 1200-nm-long device are shown in Fig. 1(b). The DC bias voltage is 0.8 V. The frequency of the AC voltage is 1 THz. It is clearly demonstrated that our deterministic Boltzmann equation solver can perform the transient simulation at such a high frequency without any numerical problem.



**Fig.1** (a) DC IV characteristics of various  $N^+NN^+$  devices, which are obtained from the deterministic Boltzmann equation solver. (b) Transient results of an  $N^+NN^+$  device whose total length is 1200 nm. The DC bias voltage is 0.8 V. AC voltages of 1 THz with various amplitudes are applied to the anode terminal. The first two periods are simulated.



## Conclusion

In this work, the transient device simulation results using a deterministic Boltzmann equation solver based on the spherical harmonics expansion has been presented. In order to avoid the numerical difficulties originated from the  $H$ -transformation, the kinetic-energy-based scheme is adopted. The numerical results demonstrate that both of DC and AC analyses can be performed without any numerical problem. It is expected that this simulator can be applied to the THz devices based on the plasma instability.

## Acknowledgements

This work was supported by Samsung Research Funding Center of Samsung Electronics under Project Number SRFC-IT1401-08. .

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**Sung-Min Hong** is an Assistant Professor with the School of Electrical Engineering and Computer Science, Gwangju Institute of Science and Technology, Gwangju, Republic of Korea.

His current research interests include deterministic Boltzmann equation solvers and simulation of terahertz devices.

For more information, please visit <https://sites.google.com/site/semidevsimlab>.



**Session A2**

**A06**

**10:20 - 10:45AM Room A June 20**

*The submitted abstract is not for publication.*

## Terahertz semiconductor devices for photonic applications

HUA LI AND JUN-CHENG CAO

Key Laboratory of Terahertz Solid State Technology, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences.

865 Changning road, Shanghai 200050, China

Email: hua.li@mail.sim.ac.cn

### Abstract

Homogeneous broadband and electrically pumped semiconductor radiation sources emitting in the terahertz regime are highly desirable for various applications, including spectroscopy, chemical sensing, and gas identification. In the frequency range between 1 and 5 THz, unipolar quantum cascade lasers employing electron inter-subband transitions in multiple-quantum-well structures are the most powerful semiconductor light sources. Here, we report the demonstration of homogeneous spectral spanning of long-cavity terahertz semiconductor quantum cascade lasers frequency comb. At a single drive current, the terahertz spectrum under radio frequency modulation continuously spans 330 GHz (~8% of the central frequency), which is the record for single plasmon waveguide terahertz lasers with a bound-to-continuum design. The homogeneous broadband terahertz sources can be used for spectroscopic applications, i.e., GaAs etalon transmission measurement and ammonia gas identification. In addition, using a fast terahertz quantum well photodetector, we successfully achieve the gigahertz modulated terahertz light detection.

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**Hua Li** is Professor of Shanghai Institute of Microsystem and Information Technology (SIMIT), Chinese Academy Sciences (CAS). He received the Ph. D degree in solid state electronics and microelectronics from SIMIT in 2009. From 2009 to 2012, he worked at the Walter Schottky Institute, Technical University of Munich in Germany as an Alexander von Humboldt research fellow. From 2012 to 2013, he worked at the Institute of Industrial Science, University of Tokyo in Japan as a JSPS postdoctoral fellow. From 2013 to 2014, he worked at the Laboratoire Matériaux et Phénomènes Quantiques, University Paris 7 in France as a postdoctoral research associate. In 2015, he was appointed as a full professor of SIMIT and selected as a fellow of “Hundred-Talent” program of Chinese Academy of Sciences. He has authored and co-authored more than 40 peer-review papers and 10 Chinese patents.



His current research interests include terahertz and mid-infrared quantum cascade laser frequency combs, active/passive mode locking of lasers, fast terahertz detection, etc.

*Session A2*

*A07*

*10:45 - 11:10AM Room A June 20*

## Making structured metals transparent for broadband electromagnetic waves

RU-WEN PENG, REN-HAO FAN, AND MU WANG

National Laboratory of Solid State Microstructures, School of Physics, and Collaborative Innovation Center of Advanced Microstructures, Nanjing University  
Nanjing 210093, China  
Email: rwpeng@nju.edu.cn

### Abstract

In this talk, we present our recent work on making structured metals transparent for broadband electromagnetic waves via excitation of surface waves. First, we theoretically show that one-dimensional metallic gratings can become transparent and completely antireflective for extremely broadband electromagnetic waves by relying on surface plasmons or spoof surface plasmons [1]. Second, we experimentally demonstrate that metallic gratings with narrow slits are highly transparent for broadband terahertz waves at oblique incidence and high transmission efficiency is insensitive to the metal thickness [2]. In the third, we significantly develop oblique metal gratings transparent for broadband electromagnetic waves (including optical waves and terahertz ones) under normal incidence [3]. Besides, the principles of broadband transparency for structured metals can be further extended to other systems [4, 5]. These investigations provide guidelines to develop many novel materials and devices, such as transparent conducting panels, antireflective solar cells, and other broadband metamaterials and stealth technologies.

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**Ruwen Peng** is a distinguished professor in Nanjing University and a principal investigator at National Laboratory of Solid State Microstructures. She has been supported by National Natural Science Funds for Distinguished Young Scholars during 2007~2010. And she was honored the Chinese Young Women Scientists' Award in 2011, and Xie Xide Award in 2013.



Her current research interests include plasmonics and nanophotonics, metamaterials, photonic quasicrystals, phononic transport and heat transfer in nanostructures.

For more information, please visit <http://microphotonics.sinaapp.com>.

**Session A2**

**A08**

**11:10 - 11:35AM Room A June 20**

## Terahertz-wave parametric wavelength conversion at room temperature

SHIN'ICHIRO HAYASHI<sup>1,2</sup>, KOUJI NAWATA<sup>2</sup>, KODO KAWASE<sup>3</sup>, HIROAKI MINAMIDE<sup>2</sup>

<sup>1</sup>NICT, 4-2-1, Nukui-Kitamachi, Koganei, Tokyo 184-8795, Japan

<sup>2</sup>RIKEN Center for Advanced Photonics, 519-1399 Aramakioba, Aoba, Sendai, 980-0845 Japan

<sup>3</sup>Graduate School of Engineering, Nagoya University, Furocho, Chikusa, Nagoya, 464-8603, Japan

Email: hayashi@nict.go.jp

### Abstract

Over the past decade, there has been remarkable growth in the field of terahertz frequency science and engineering, which has become a vibrant, international, cross-disciplinary research activity. Wavelength conversion in nonlinear optical materials is an effective method for generating and detecting coherent terahertz waves owing to the high conversion efficiency, bandwidth, wide tunability, and room-temperature operation, and if the tuning range and the peak power can be enhanced, drastic developments in basic researches and industrial applications can be expected.

Here we demonstrate the generation of high-brightness terahertz waves using parametric wavelength conversion in a nonlinear MgO doped LiNbO<sub>3</sub> crystal. We revealed novel parametric wavelength conversion process using stimulated Raman scattering in MgO:LiNbO<sub>3</sub> without stimulated Brillouin scattering using recently-developed microchip Nd:YAG laser. We also demonstrated the coherent detection of generated terahertz waves using nonlinear up-conversion.

A number of applications require high brightness, that is, intense and narrowband, terahertz waves such as observing multi-photon absorption to specific excitation states. We speculate that the high-brightness terahertz wave and its visualization could be powerful tools not only for solving real world problems but also fundamental physics. We expect that these methods will open up new fields and tune up killer applications.

### Acknowledgements

The authors would like to thank Prof. T. Taira of IMS, Dr. Sakai of Hamamatsu Photonics, all of previous and present team members, Prof. H. Ito of RIKEN and Prof. M. Kumano of Tohoku University for useful discussions. This work was partially supported by Collaborative Research Based on Industrial Demand of the Japan Science and Technology Agency (JST), and JSPS KAKENHI Grant Numbers 25220606, 25286075, and ImPACT Program of Council for Science, Technology and Innovation.

**Shin'ichiro Hayashi** received the Ph.D. degree in physics from Meiji University, Japan, in 2004. From 2004, he was with RIKEN, Japan, as a Researcher. In 2016, he joined the National Institute of Information and Communications Technology, as a Senior Researcher. His research interests include bright terahertz wave generation and coherent detection using nonlinear optics and their application.





*Session A2*

*A09*

*11:35 - 12:00 PM Room A June 20*

## Development of Small Size Terahertz Vacuum Sources in IECAS

WENXIN LIU, CHAO ZHAO, XIN GUO

Institute of Electronics, Chinese Academy of Sciences, Beijing, China

Email: lwenxin@mail.ie.ac.cn

### **Abstract**

Terahertz frequencies are among the most under developed electromagnetic spectra, even though their potential applications are promising in biochemical sensing, imaging for medical and security applications, astrophysics and remote atmospheric monitoring, and high-bandwidth communications. Among their wide applications, the lightweight, low voltage and broadband sources of high-power coherent THz radiation are important for military radar, electronic countermeasure systems and communications [1]. Vacuum electronic devices [2]-[5] such as the traveling wave tube amplifier (TWTA), backward wave oscillator and extended interaction oscillator show great potential for applications at the frequency because of wide band and high power. At THz band, the most critical part of small size THz vacuum sources is the slow wave structure, which determines the output performances, such as the output power and signal band. In the millimeter and sub-millimeter wave vacuum devices, the various of SWSs including coupling cavity, disk-loaded, helix and complex CC are used. However, they are not suitable for the THz band, resulting from the difficulty of fabricating and integrating.

Folded waveguide (FW) or serpentine circuits, for example, have ~10:1 aspect ratio in the waveguide height dimension. This is much larger than the ideal for both machining, which is limited by the length of the tool shank with acceptable wobble; and photolithography, which is limited by defocusing and absorption of light as it penetrates into deep photoresist. These requirements are the topic of ongoing research in the vacuum electronics community, motivated by the continued interest in high power mm-THz sources. Consequently, there is a great interest in the study and development of FW SWS. For the satisfied with requirement of high speed communication and ViSAR, the TWT has been developed. Based on the FW, the small size THz vacuum devices are developed in China, including UESTC, IECAS CETC 12 and CAEP, etc. In this talk, we report the development of small size THz vacuum devices in IECAS.

At IECAS, three kinds THz devices have been developed, such as the 0.3THz EIO, the peak power exceeds 4W. The 0.1THz EIO generates the output power is larger than 12W. Moreover, the THz TWT has been developed through the small size electron gun, high strength focusing magnetic field and high frequency structure welding. It produces the output power exceeds 2W and the band width is larger than 5GHz. Now we are developing the continued wave TWT for the power exceeds 10W and signal band width larger than 5GHz.

**Wenxin Liu** is Associate Professor of Institute of electronics, Chinese Academy of Sciences. He is a Senior member of IEEE society. He was the recipient of the progress prize in military scientific and technology for his contributions to the field of THz devices in 2007, 2012 and 2016.

His current research interests include terahertz sources, high power microwave, and free-electron laser.



*Session A2*

*A10*

*12:00 - 12:25 PM Room A June 20*

## Recent Progress of Terahertz Detection Based on Two-dimensional Materials

CHANGLONG LIU, WEIWEI TANG, LIN WANG\*

National Laboratory for Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, 200083, Shanghai, China

Email: wanglin@mail.sitp.ac.cn

### Abstract

Recent years, layered van der Waals crystals consist of individual atomic planes weakly coupled by vdW interaction have attract great interests due to their intriguing physical properties, such as superconductivity, high carrier mobility, topologically protected surface states and among many others. An ambitious practical goal is to exploit planes of vdW crystals as building blocks of more complex optoelectronic application, especially in the terahertz band. The pursuit of two-dimensional materials for terahertz detection is promoted by the unique properties beyond traditional system, such as good CMOS-compatibility, easy for fabrication and fast response. Especially, graphene can support terahertz plasmon which can lead to enhanced THz absorption. Graphene-based terahertz detectors rely on the photothermoelectric and self-mixing effects [1][2], both of these effects depends on the near-field or the decay of plasmons. Also, other two-dimensional materials such as black phosphorus, topological insulator exhibit exotic THz optoelectronic properties, such as anisotropic band structure in BP, interplay between surface states and bulk states in Bi<sub>2</sub>Se<sub>3</sub>[3].

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**Lin Wang** is an Associate Professor of Microelectronics in Shanghai Institute of Technical Physics, CAS. He is a member of Youth Promotion Association, CAS. He was the recipient of many prizes including special prize of president scholarship. Outstanding achievement award in Shanghai. He has authored or coauthored more than 40 technical journal papers and conference presentations.



His current research interests include plasma wave detection of terahertz radiation using graphene and GaN, simulation and modeling of carbon-based nanomaterials and devices, graphene-like two-dimensional optoelectronics. Email: [wanglin@mail.sitp.ac.cn](mailto:wanglin@mail.sitp.ac.cn).

**Session A3**

**A11**

**14:00 - 14:25PM Room A June 20**

## 300GHz wireless link with a CMOS transceiver

MINORU FUJISHIMA

Graduate School of Advanced Sciences of Matter, Hiroshima University

1-3-1 Kagamiyama, Higashi-hiroshima, Japan

Email: fuji@hiroshima-u.ac.jp

### Abstract

Since terahertz provides a wide frequency band, terahertz communication realizes a data rate exceeding 100 Gbps approaching fibre-optic speed. The frequency band from 252 to 275 GHz has already been allocated for communication. Further discussion is being made to use the frequency band exceeding 275 GHz, which has not been assigned yet, for communication use. On the other hand, since terahertz has large atmospheric attenuation and strong directivity, it is limited to short-distance fixed radio communication. However, it is long-distance and mobile application that is intrinsically expected for wireless communication. In this talk, even in terahertz, it is shown that kilometre communication is potentially possible by selecting the frequency appropriately. It is also shown that terahertz communication can be performed using CMOS process, which was said to have inferior high frequency characteristics to compound semiconductors. How will the world change when technologies beyond such conventional common sense are established? The impact of terahertz communication and the contribution of CMOS transceivers are discussed.

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**Minoru Fujishima** received the B.E., M.E. and Ph.D degrees in Electronics Engineering from the University of Tokyo, Japan in 1988, 1990 and 1993, respectively. He joined faculty of the University of Tokyo in 1988 as a research associate, and was an associate professor of the School of Frontier Sciences, University of Tokyo in 1999. He was a visiting professor at the ESAT-MICAS laboratory, Katholieke, Universiteit Leuven, Belgium, from 1998 to 2000. He has been a professor of the Graduate School of Advanced Sciences of Matter, Hiroshima University since 2009.



He studied design and modeling of CMOS and BiCMOS circuits, nonlinear circuits, single-electron circuits, and quantum-computing circuits. His current research interests are in integrated devices and systems for terahertz communication and sensing. He coauthored more than 50 journal papers and 120 conference papers. He served as a distinguished lecturer in IEEE solid-state circuits society from 2011 to 2012. He is senior members of IEEE and IEICE (Japan).

**Session A3**

**A12**

**14:25 - 14:50PM Room A June 20**

## **Surface Plasmon enhanced Sub-THz CMOS detectors**

Z. SHEN, C. ZHANG, Q. LOU, R. WU, B. JIN, F. YAN AND X. JI,

School of Electronic Science and Engineering, Nanjing University, Nanjing 290031, China.

Phone/Fax: +86-25-83593965

Email: xji@nju.edu.cn; fyan@nju.edu.cn

### **Abstract**

Surface plasmon Resonances (SPR) antenna has aroused considerable interest in the field of terahertz research owing to its extraordinary light concentration capacity. This paper focuses on the design of silicon material based SPR antenna for CMOS Terahertz detector. Computer Simulation Technology has been used to predict antenna resonance frequencies, local field enhancements and distributions. The designed antenna structures at 0.65THz are then integrated with CMOS terahertz detector. The experimental results show that by combining with Si SPR antennas, the maximum voltage responsivity of CMOS terahertz detector can be boosted by up to 17 times due to the increased field concentration in the channel area of MOSFETs. The antenna design with plasmonic effects provides a technology platform for the ease of design and fabrication of CMOS THz detectors.

**Keywords:** Surface Plasmon Resonances, CMOS Terahertz detector, Voltage response, Antenna

**Xiaoli Ji** is Professor in the college of Electronic Science and Engineering at Nanjing University. She received her BS (1993) in Physics from Jilin University (China) and PhD (1998) from Tsukuba University (Japan). Before joining Nanjing University (2009), she held various research positions at Tsukuba University, Kyoto University and Victor Company of Japan. At Nanjing University, Dr. Xiaoli Ji has developed some vigorous research programs in CMOS Si devices physics and reliability. Recently, her group focuses on the development of CMOS THz detectors that have unique structures and useful properties for applications. During last five years, She has published more than 30 peer-reviewed journal articles, submitted 13 patents and has received several research fundings from various agencies.



For more information, please visit <http://ese.nju.edu.cn/faculty.php?name=jixiaoli&lang=cn>



## Session A3

A13

14:50 - 15:15PM Room A June 20

## Photonic crystal cavity optomechanics for the applications of low phase noise frequency source and high-performance sensing

YONGJUN HUANG, GUANGJUN WEN

School of Communication and Information Engineering, University of Electronic Science and Technology of China, Chengdu, 611731, China

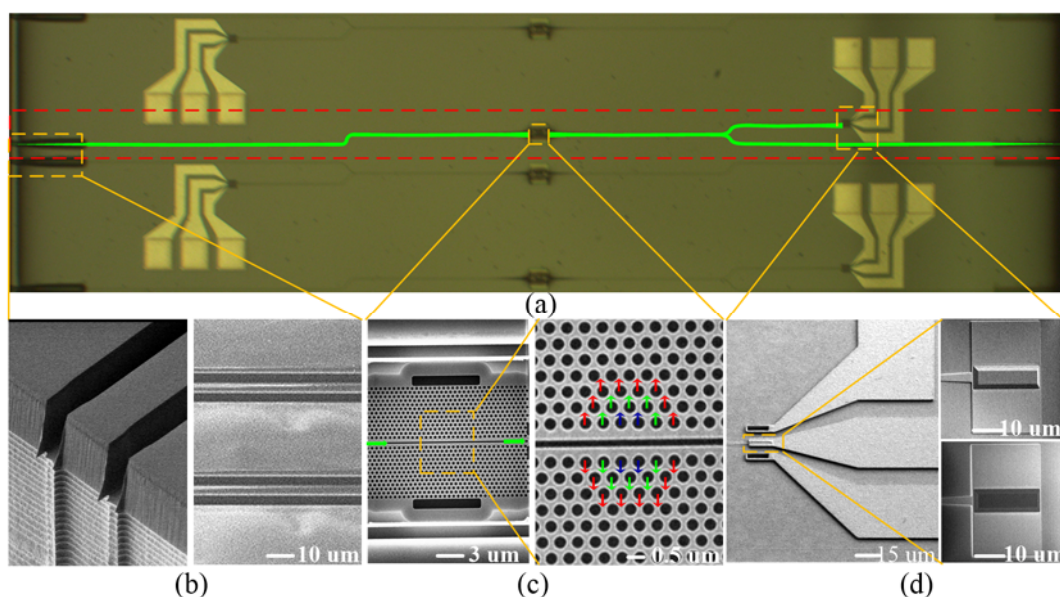
Email: yongjunh@uestc.edu.cn

CHEE WEI WONG

Fang Lu Mesoscopic Optics and Quantum Electronics Laboratory, University of California at Los Angeles, Los Angeles, CA 90095, USA

**Abstract**

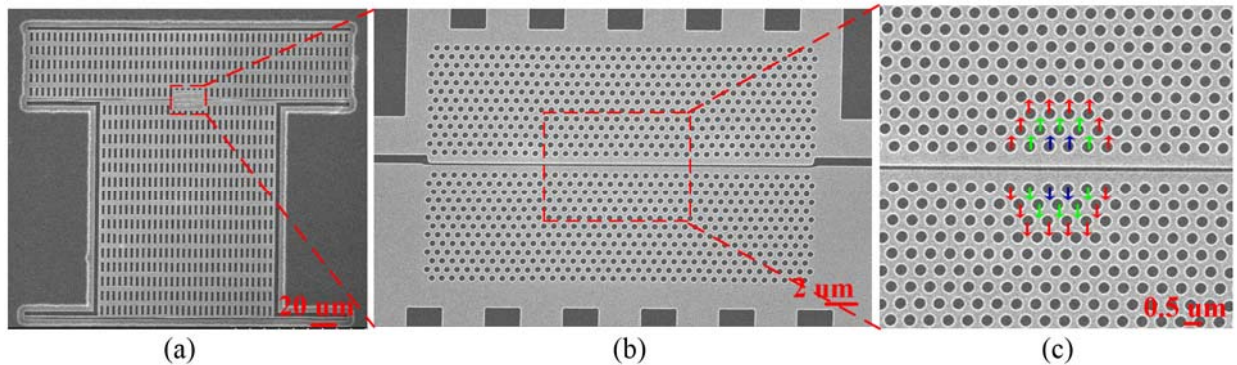
Based on the air-slot line-defected photonic crystal nano-cavity [1], here we develop a monolithic integration of photonic crystal optomechanical oscillators and on-chip high speed Ge detectors (see Fig. 1) by using the silicon CMOS platform. With the generations of both high harmonics (up to 59th order) and subharmonics (down to 1/4), due to strong mutual couplings between optomechanical self-sustained oscillation and self-pulsation oscillation, our chipset provides multiple low phase noise frequency tones [2] for applications in both frequency multipliers and dividers. The synchronization between two mechanical modes [3] and dynamical chaos [4] in the optomechanical cavity are reported as well. These characteristics enable optomechanical oscillators as a frequency reference platform for radio-frequency-photonic information processing.



**Fig.1** Fabricated optomechanical cavity integrated with on-chip Ge-detector

Moreover, we further demonstrate a chip-scale optomechanical cavity with large mass (see Fig. 2) which operates at  $\sim 77.7$  kHz fundamentally and exhibits large optomechanical coupling of 44+ GHz/nm.

The mechanical shifting range of  $\sim 58$  kHz and more than 100-order harmonics are obtained with which the free-running frequency instability is lower than  $10^{-6}$  at 0.1 sec integration time [5]. The optomechanical coupling strength can be mechanically controlled by taper fiber and the Drude self-pulsation plasma locking is also reported in this platform [6]. Such large mass optomechanical cavity can be applied for the sensing applications, such as accelerometers and magnetometers.

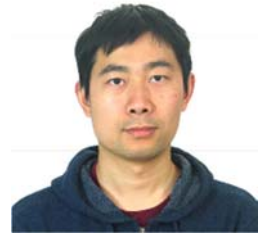


**Fig.2** Fabricated large mass optomechanical cavity

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**Yongjun Huang** received the M.S. and Ph.D degrees from University of Electronic Science and Technology of China (UESTC) in 2010 and 2016 respectively. He is currently the assistant Professor with UESTC. He was a visiting scholar with the Solid-State Science and Engineering, and Mechanical Engineering, Columbia University, and a visiting project scientist with the Electrical Engineering, University of California at Los Angeles (UCLA). He is a Member of IEEE and OSA.



His current research interests include the fundamentals of chip-scale cavity optomechanics and metamaterials, and the applications for low phase noise RF sources and high-performance force/field sensors.

For more information, please visit:

<https://sites.google.com/site/yongjunhuangresearchhomepage/home>.

## Session A3

A14

15:15 - 15:40PM Room A June 20

## Fast THz Modulator based on the stagger-netlike GaN HEMT active metamaterial

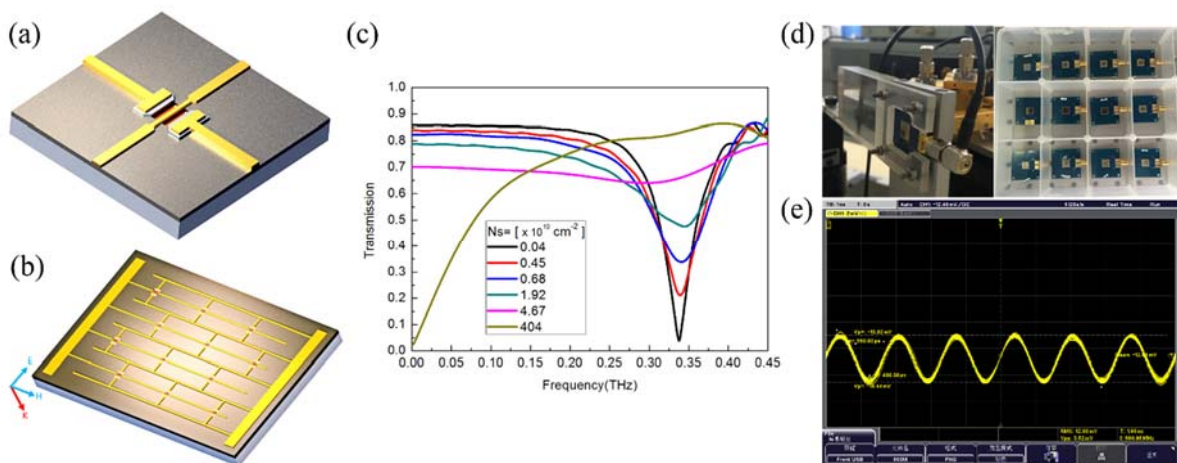
YUNCHENG ZHAO<sup>1</sup>, YAXIN ZHANG<sup>1\*</sup>, SHIXIONG LIANG<sup>2</sup>, ZHIHONG FENG<sup>2</sup> AND ZIQIANG YANG<sup>1\*</sup><sup>1</sup>Terahertz Science Cooperative Innovation Center, University of Electronic Science and Technology of China No.4, Section 2, North Jianshe Road, Chengdu, 610054, China<sup>2</sup>National Key Laboratory of Application Specific Integrated Circuit, Hebei Semiconductor Research Institute, Hezuo Road, Shijiazhuang, 050051, China.

Email: \*zhangyaxin@uestc.edu.cn

Email: \*zqyang@uestc.edu.cn

**Abstract**

Terahertz technology promises unique applications in high speed communication, high accuracy imaging and so on [1]. However, one major bottleneck for developing Terahertz application systems is the lack of high-performance dynamic devices for effectively manipulating the Terahertz wave. In recent years, the rapid development of two-dimensional electron gas (2DEG) devices provides a promising way to develop dynamic terahertz devices [2]. In this paper, we combined a stagger-netlike metamaterial array with high-electron-mobility transistor (HEMT) structure to form a electronic grid-controlled THz modulator. By controlling the carrier concentration of 2DEG, the mode conversion between two kinds of dipolar resonances has been realized. Modulation depth of this device can reach up to 94%. More importantly, in the dynamic test, 600 MHz sinusoidal signals was received by a THz detector. It may provide a way to achieve effective active devices in THz wireless communication system.



**Fig.1** (a) 3-D structure of a GaN HEMT metamaterial unit cell. (b) Schematic of the THz modulator. (c) Simulation transmission spectrum results with different carrier density. (d) Image of packaged THz modulator. (e) The received sinusoidal modulating signals.

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**Yaxin Zhang** is Professor and doctoral supervisor of University of electronics science and technology of China. Prof. Zhang received the B.Sc. in SiChuan university and Ph.D. degrees in University of Electronic Science and Technology of China(UESTC) in 1999 and 2009, respectively. In April 2006 he joined the THz science and technology research center of UESTC.



Currently, he is secretary general of THz society of CIE and associate director of the Sichuan Key Laboratory of THz science and Technology. He was selected in the Program for New Century Excellent Talents in University of Ministry of Education of China in 2013 and Sichuan province outstanding youth academic leaders scheme in 2014.

He has published over 60 SCI journal papers in Nano Letters, Physical Review Letters, Applied Physics Letters, Physical Review, IEEE Transactions, etc. His research interests include THz radiation sources, THz functional device and THz wireless communication.

Phone Number (M):+86-18980677112

Phone Number (O):+86-28-83202603

E-mail: [zhangyaxin@uestc.edu.cn](mailto:zhangyaxin@uestc.edu.cn)

**Session A4**

**A15**

**16:00 - 16:25PM Room A June 20**

## Hydration of various solutions observed by terahertz spectroscopy

TOSHIAKI HATTORI

Division of Applied Physics, Faculty of Pure and Applied Sciences, University of Tsukuba

Email: hattori@bk.tsukuba.ac.jp

### Abstract

Use of terahertz waves for sensing various type of materials has been an important subject of research. The target materials include biological tissues, various kind of liquids, industrial products, etc. In most of cases, water is the most important absorber of terahertz waves. It is crucial, therefore, to understand the terahertz absorption properties of water in various situations.

It is known that the terahertz absorption of water is strongly affected by the interaction with other molecules in solutions, gels, crystals, or other types of phases. In aqueous solutions, for example, the solute is stabilized by the interaction with surrounding water molecules, and the water molecules incorporated in this interaction are very often strongly bound to the solute, leading to reduced mobility and reduced terahertz absorption.

We have constructed a high-precision terahertz time-domain spectroscopy apparatus for hydration study. Results of hydration study of protein (hen egg white lysozyme) aqueous solution with several ammonium salts [1,2] is briefly described below. Terahertz absorption coefficient of the protein-salt aqueous solutions and salt aqueous solutions were obtained as a function of the salt concentration. The difference between the results of protein-salt aqueous solutions and those of salt aqueous solutions exhibits the nature of the hydration water of the protein and also the effect of salt on them. It was found that the hydration layer of the protein is affected by ions (mostly anions) added to the solution, and that so-called kosmotropic ions (structure makers), such as sulfate ion, reduce the amount of immobile hydration water, whereas chaotropic ions (structure breakers), such as thiocyanate ions, increase it. It is shown that the dynamical properties of hydration water molecules is correlated with the stability of the macromolecules, whereas their density with the solubility.

Measurements on other types of water-rich systems have shown that the mobility of water sometimes increases after hydration, or that the hydration number changes drastically upon a small change in the concentration. Study of hydration using terahertz waves is expected to produce fruitful results in various fields including solution chemistry, sol-gel science, biology, and medicine.

### Reference

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**Toshiaki Hattori** is Professor at Division of Applied Physics, Faculty of Pure and Applied Sciences, University of Tsukuba. He is a Member of the Japan Society of Applied Physics, the Spectroscopical Society of Japan, the Physical Society of Japan, and Japan Society for Molecular Science. He is a representative of the Japan Society of Applied Physics, a committee member of the Division of Terahertz Spectroscopy, the Spectroscopical Society of Japan, and a councilor of Terahertz Technology Forum.



His current research interests include terahertz spectroscopy of bio-related materials and development of terahertz sensing devices.

For more information, please visit <http://www.bk.tsukuba.ac.jp/~hattori/>.



**Session A4**

**A16**

**16:25 - 16:50PM Room A June 20**

## Ultra-broadband Wireless Communications in the 0.1-10 Terahertz Band

CHONG HAN

University of Michigan–Shanghai Jiao Tong University Joint Institute

Shanghai Jiao Tong University, China

Email: chong.han@sjtu.edu.cn

### **Abstract**

By supporting tens or hundreds GHz bandwidths, Terahertz (THz)-band (0.1-10 THz) communication is envisioned as a key wireless technology of the next decade. The THz band will help overcome the spectrum scarcity problems and capacity limitations of current wireless networks, by providing an unprecedentedly large bandwidth. In addition, THz-band communication will enable a plethora of long-awaited applications, both at the nano-scale and at the macro-scale, ranging from wireless massive-core computing architectures and instantaneous data transfer among non-invasive nano-devices, to ultra-high-definition content streaming among mobile devices and wireless high-bandwidth secure communications.

In this invited speech, an overview of THz-band communications will be provided. First, the current progress and open research directions in terms of THz-band channel modeling will be presented. The main phenomena affecting the propagation of THz signals will be explained and their impact on the channel capacity will be assessed. Second, novel communication mechanisms such as the modulation techniques, resource allocation, timing acquisition schemes, and Ultra-Massive Multiple-Input Multiple-Output (UM- MIMO) will be presented. Finally, the state of the art and open challenges in the network layer design and other relevant research directions will be stated. This presentation is expected to provide the audience with the necessary knowledge to work in a cutting-edge research field, at the intersection of antennas and propagation, and information and communication technologies.

**Chong Han** received the Bachelor of Engineering degree in Electrical Engineering and Telecommunications from The University of New South Wales (UNSW), Sydney, Australia, in 2011. He obtained the Master of Science and the Ph.D. degrees in Electrical and Computer Engineering from Georgia Institute of Technology, Atlanta, GA, USA, in 2012 and 2016, respectively. Since June 2016, he is an Assistant Professor, Associate Special Research Fellow and PhD advisor with the University of Michigan–Shanghai Jiao Tong University Joint Institute, Shanghai Jiao Tong University, Shanghai 200240, China. He has been mentoring several undergraduate and graduate students. Dr. Han was the recipient of Shanghai Sailing Program award in 2017, the Australia's Commonwealth Scientific and Industrial Research Organization (CSIRO) Scholarship in 2010-2011, and the National Information Communications Technology Research Centre (NICTA) of Excellence Summer Scholarship, Australia in 2009-2010.



His current research interests include Terahertz Band Communication Networks, Electromagnetic Nanonetworks, 5G Cellular Networks. In these areas, he has published multiple peer-reviewed scientific publications, in prestigious journals and top-rated conferences in IEEE and ACM. He has been an editor of Elsevier Nano Communication Networks journal and IEEE Access since 2016, and served as a member of the technical program committees of multiple IEEE and ACM international. He is a member of the IEEE.

Webpage: <http://umji.sjtu.edu.cn/~chan/>

Google Scholar: <https://scholar.google.com/citations?user=nfbP5VkAAAAJ&hl=en&oi=ao>

**Session A4**

**A17**

**16:50 - 17:15PM Room A June 20**

## Millimeter- and terahertz-wave technology for communication and radar/imaging applications by photonics technology

ATSUSHI KANNO

National Institute of Information and Communications Technology, Japan

Email: kanno@nict.go.jp

### **Abstract**

Advanced optical fiber communication technologies enable low-loss and broad-bandwidth transmission in the millimeter-wave and terahertz-wave bands via an optical fiber network. Precise optical modulation techniques can directly generate the millimeter-wave signals, and finally, an optical frequency comb signal generated by the modulation also provides the terahertz-wave signals by optical heterodyning systems. These technologies on the signal generation could be utilized for realization of distributed antenna system in the millimeter- and terahertz-wave bands based on the optical fiber network for some specific applications: foreign object debris detection systems for airport runway surveillance and high-speed railway radiocommunication systems between train and trackside. In the talk, we briefly introduce the R&D activities on the millimeter- and terahertz-wave for both wireless communication and radar/non-destructive imaging systems based on photonics.

**Keywords:** Terahertz-wave, optical frequency comb, optical modulation, FOD detection system, train communication system

**Dr. Atsushi Kanno** received B.Sci., M.Sci., and Ph.D. degree in science from the University of Tsukuba, Japan, in 1999, 2001, and 2005, respectively. In 2005, he was with the Venture Business Laboratory of the Institute of Science and Engineering, University of Tsukuba. In 2006, he joined the National Institute of Information and Communications Technology (NICT), Japan. His research interests are microwave/millimeter-wave/terahertz photonics, ultrafast optical and radio communication systems, lithium niobate optical modulators, and ultrafast phenomena in semiconductor optical devices. He is a member of the Institute of Electronics, Information and Communication Engineers (IEICE), the Japan Society of Applied Physics (JSAP), the Laser Society of Japan, and the Institute of Electrical and Electronic Engineers (IEEE).



Session A4

A18

17:15 - 17:40PM Room A June 20

# ECP: Error Control with Probing for Electromagnetic Nanonetworks with Energy Harvesting

XIN-WEI YAO, DE-BAO MA

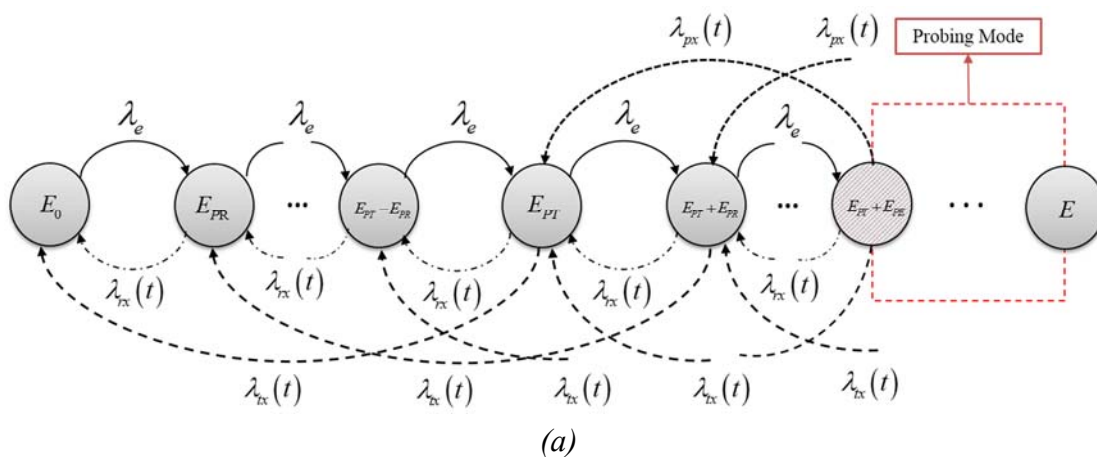
College of Computer Science and Technology  
Zhejiang University of Technology, Hangzhou, China  
Email: xwyao@zjut.edu.cn, dbma@zjut.edu.cn

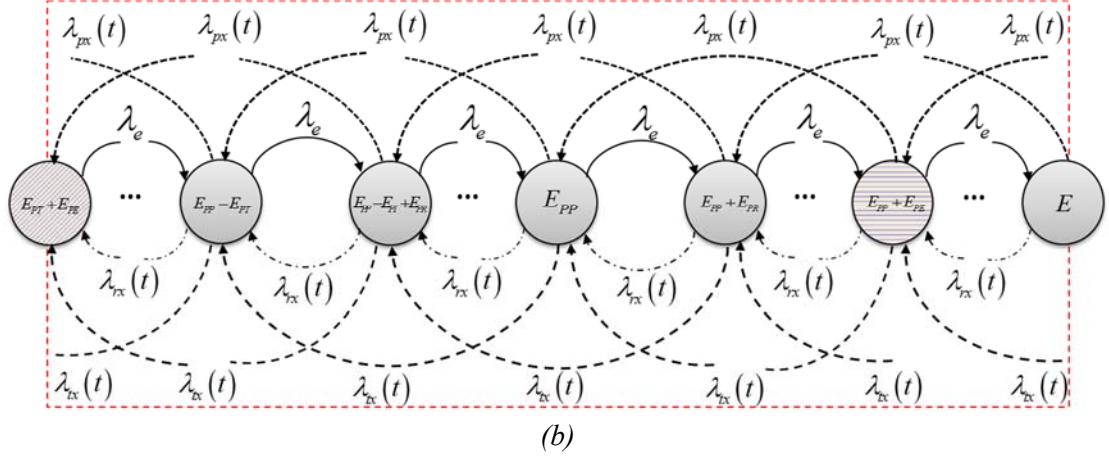
MENG-NA ZHANG, CHAO-CHAO WANG

College of Computer Science and Technology  
Zhejiang University of Technology, Hangzhou, China  
Email: mnzhang@zjut.edu.cn, ccwang@zjut.edu.cn

## Abstract

Nanonetworks consist of nano-scale communicating devices, which can only perform some simple tasks such as computing, data storage and processing at the nanoscale. The major challenges in nanonetworks are posed by the very limited energy storage and the high error-prone wireless links as a result of severe path loss in Terahertz band (0.1-10 THz). Therefore, efficient and effective error control mechanisms are required for nanonetworks [1-3]. In this paper, firstly, a novel error control mechanism with probing mode (ECP) for nanonetworks with energy-harvesting system is proposed. In particular, each packet will be transmitted only after one probing packet is transmitted successfully. Secondly, the corresponding mathematical model of the energy harvesting-consumption process is developed based on the extended Markov chain. With the proposed energy model, the energy consumption of each transmitting state and its probability distribution are comprehensively investigated. Finally, numerical results are provided to evaluate the performance of the proposed ECP with different metrics, including end-to-end packet delay, end-to-end packet delivery probability and the achievable throughput. The results show that the proposed ECP improves the energy utilization and decreases the packet error rate.





**Fig.1** Energy model of the energy harvesting-consumption process based on Markov chain.

**Table 1** The list of notation

Symbol	Description
$\{E\}$	The energy state when the energy value is $E$ .
$E_0$	Initial energy value.
$E_{PR}$	The energy value of receiving a feedback or receiving a packet, which is supposed as the data receiving energy threshold $\tau$ .
$E_{PT}$	The energy value of sending a packet, which is supposed as the data sending energy threshold $\gamma$ .
$E_{PE}$	The total energy value of sending a probing packet and receiving a
$E_{\max}$	Energy saturation value.
$E_{PP}$	An energy value between $E_{PT} + E_{PE}$ and $E$ .
$E_{PT} + E_{PE}$	Suppose the probing mode energy threshold is $\delta$ .
$\lambda_e$	Energy-harvesting rate.
$\lambda_{rx}(t)$	The probability of receiving data packets.
$\lambda_{px}(t)$	The probability of sending probing packets
$\lambda_{tx}(t)$	The probability of sending data packets.

The proposed ECP for EM nanonetworks operates as follows. Each nanonode will enter the probing mode only as the energy value is beyond the energy threshold  $\delta = E_{PT} + E_{PE}$ . In the probing mode, one probing packet will be transmitted to detect the channel conditions at first. Then data packet will be transmitted only after the probing packet is transmitted and received successfully and the remained energy is still beyond the energy threshold  $\gamma = E_{PT}$ .

The mathematical model for the energy harvesting-consumption process based on extended Markov chain is shown in Fig.1. In the Fig.1, each state in the energy model corresponds to an energy state of nanonode. The dashed box in Fig.1(a) refers to a set of states that the nanonode belongs to the probing mode, which is detailed described in Fig.1(b). The solid lines represent the energy harvesting process

while the dotted lines represent the energy consumption process. The short dashed lines represent the energy consumption processes of sending probing packet or receiving its feedback. The long dotted lines represent the energy consumption processes of sending data packet or receiving its feedback.

In detail, two cases in the model of the energy harvesting-consumption process based on Markov chain are described as follows:

Case 1: The process of energy harvesting operates as follows: nanonode keeps harvesting energy without sending or receiving any packet from the initial energy state  $\{E_0\}$  to the saturation energy state of  $\{E_{\max}\}$ .

Case 2: The process of energy harvesting and data transmission operates as follows: from the beginning of initial energy state  $\{E_0\}$ , the nanonode keeps harvesting energy and receiving packets, but it does not send any packet. After at the state  $\{E_{PT} + E_{PE}\}$ , there are two conditions:

CONDITION 1: The mode of energy harvesting and data reception: nanonode keeps harvesting energy and receiving packets without sending packets until the nanonode reaches the maximum energy and enters the energy saturation state.

CONDITION 2: Probing mode: nanonode keeps harvesting energy and receiving packets.

In addition, as the nanonode wants to send data packet in a certain state like  $\{E_{PP} + E_{PE}\}$ , it will enter into the probing mode. In the probing mode, nanonode will firstly send out one probing packet to detect the channel condition, and then receive the corresponding feedback. As a result, nanonode consumes the energy of  $E_{PE}$  and enters into the energy state of  $\{E_{PP}\}$ . According to the feedback of the probing packet, there are two cases:

If the feedback is a NAK or timeout, i.e., the channel is in bad condition, nanonode needs to retransmit the probing packet until reaches the maximum retransmission time. Note, it is necessary to determine whether the total energy of the nanonode is beyond the energy threshold  $\delta$  every time before detecting the channel. If so, it means that the energy is sufficient for channel detection and the probing packet can be send out. The probing is continued until an ACK is received or the maximum number of detection is reached. If not, the nanonode needs to harvesting energy until beyond the energy threshold  $\delta$ , and then channel detection is performed.

If the feedback is an ACK and the energy in nanonode is beyond the energy threshold  $\gamma$ , then one packet will be transmitted. This process will consume the energy of  $E_{PT}$ , and let the nanonode move to the state of  $\{E_{PP} - E_{PT}\}$ . It will enter into the probing mode again as soon as the feedback is NAK or the timeout is received.

**References**

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- [3] Akkari, N, et al. "Joint physical and link layer error control analysis for nanonetworks in the Terahertz band." *Wireless Networks*, 22.4 (2016): 1221-1233.



**Xin-Wei Yao** is an Associate Professor with the College of Computer Science and Technology at the Zhejiang University of Technology, Hangzhou, China. He is a Member of IEEE and ACM. He is the Steering Committee member of the Eleventh International Conference on Quantum Nano/Bio, and Micro Technologies (ICQNM 2017). He was the recipient of the Distinguished Associate Professor Award and the Outstanding Doctoral Thesis Award at the Zhejiang University of Technology. He has been rated the outstanding Peer Reviewer of Computer Science for his contributions in 2016.



From March 2012 to February 2013, he was a visiting scholar at the Loughborough University, Leicestershire, UK. From August 2015 to July 2016, he was a visiting professor at the University of Buffalo, The State University of New York, Buffalo, NY, USA. He has served on program and organizing committees for many international conferences. He is a Member of IEEE and ACM. He has published more than 40 peer-reviewed papers, and the publications appear in leading publication venues in wireless communication research.

His current research interests are in the area of Terahertz-Band Communication Networks, Electromagnetic Nanonetworks, Wireless Ad Hoc and Sensor networks, Wireless Power Transfer and the Internet of Things.

For more information, please visit <http://www.escience.cn/people/xwyao/index.html>

**Session A4**

**A19**

**17:40 - 18:05PM Room A June 20**

## Terahertz waveguide filters based on periodic structures

YA-XIAN FAN, LU ZHANG, ZHI-NAN JIANG,

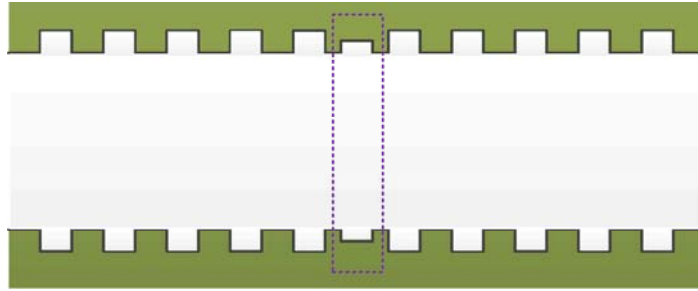
Key Lab of In-fiber Integrated Optics, Ministry Education of China,  
Harbin Engineering University, Harbin 150001, People's Republic of China  
Email: yxfan@hrbeu.edu.cn

ZHI-YONG TAO

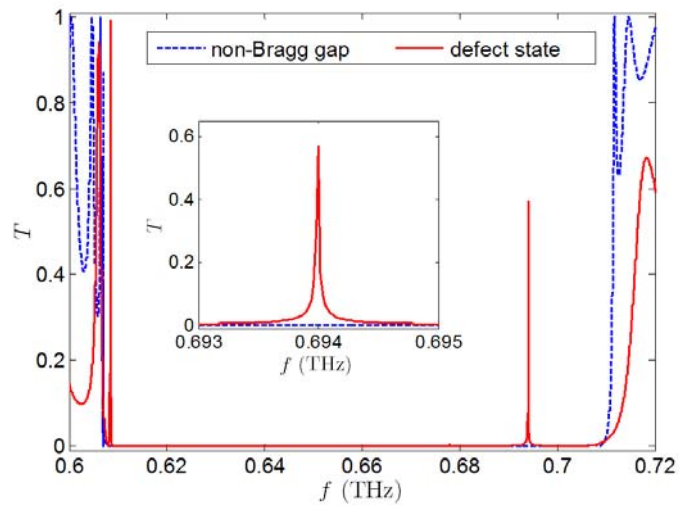
Physics Research Center, College of Science  
Harbin Engineering University, Harbin 150001, People's Republic of China  
Email: zytiao@hrbeu.edu.cn

### Abstract

Terahertz (THz) filters has attracted great interests because of their essential applications in various THz systems [1]. Instead of the weak response natural materials, many artificial structures and materials have been applied to demonstrate THz filter effects [2-5]. However, most of filters have been developed for spatial THz radiation except a few waveguide filters [6, 7]. Here, we propose a terahertz (THz) narrow band filter of waveguide type by inserting a straight tube into a ten-period corrugated waveguide. The periodically corrugated tube wall can always lead to various pass and stopbands in the transparent spectrum. In both Bragg and non-Bragg stopbands, terahertz wave cannot propagate [8]. When we inserted a straight tube into a perfect period waveguide, an unexpected transparency appears in the non-Bragg frequency gap. The waveguide structure is shown in Fig. 1, where a defect is denoted by the purple frame. On the both side of the defect, there are five periods of the corrugated THz tubes. Using the finite element method with COMSOL Multiphysics, we calculated the transmission of the waveguide structures with and without defect, which are shown in Fig. 2 by the solid and dashed lines, respectively. It is clear that there is an extraordinary transmission in the former non-Bragg gap when the defect is inserted. To clearly identify the filter effect, we enlarged the transmitted peak and depict it in the insert. Furthermore, the peak is extremely narrow to be a good candidate for THz filtering. Our findings provide a terahertz waveguide filter based on non-Bragg gaps of periodic structures. The proposed structure will benefit the THz system for future applications.



**Fig.1** Waveguide filter with a defect inserted in period structures.



**Fig.2** Transmission spectrum of defect state. The insert is the enlarged view of the filter peak.

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**Ya-Xian Fan** is Professor of the College of Science, Harbin Engineering University, Harbin, China. She is currently a Director of Opto-Electronic-Mechanical Technology & System Integration Chapter of China Instrument and control Society and a Committee Member of Opto-Electronic Technology Professional Committee of the Chinese Optical Society. She is also a Senior Member of the Chinese Optical Society. She was awarded New Century Excellent Talents from University of Ministry of Education of China, in 2008.



Her current research interests include microstructure terahertz waveguide devices, optical waveguides, mode field regulations, microstructure fiber photonics, all-optical logical devices, and nonlinear signal processing.

For more information, please visit: <http://homepage.hrbeu.edu.cn/web/fanyaxian>.

**Session B1**

**B01**

**8:00 - 8:25 AM Room B June 20**

## Epitaxial Growth of Two-Dimensional Layered Transition-Metal Dichalcogenides and Heterostructures for 2D-Electronics

YUMENG SHI

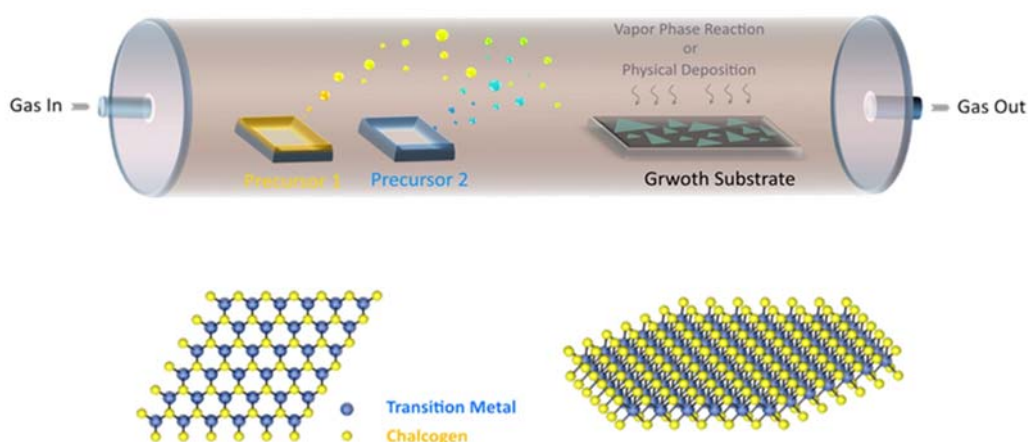
International Collaborative Laboratory of 2D Materials for Optoelectronics Science and Technology,  
College of Optoelectronic Engineering, Shenzhen University

Shenzhen 518060, China.

Email: Yumeng.shi@szu.edu.cn

### Abstract

Recently there have been many research breakthroughs in two dimensional (2D) materials including graphene, boron nitride (h-BN), black phosphors (BP) and transition metal dichalcogenides (TMDCs). The unique electrical, optical, and thermal properties in 2D materials are associated with their strictly defined low dimensionalities. These materials provide a wide range of basic building blocks for next generation electronics. The chemical vapor deposition (CVD) technique has shown great promise to generate high-quality TMDC layers with scalable size, controllable thickness and excellent electronic properties suitable for both technological applications and fundamental sciences. The capability to precisely engineer 2D materials by chemical approaches has also given rise to fascinate new physics which could lead to exciting new applications. In this talk, we introduce the latest development of TMDC synthesis by CVD approaches and provide further insight for the controllable and reliable synthesis of atomically thin TMDCs. Understanding on the vapor phase growth mechanism of 2D TMDCs could benefit the formation of complicated heterostructures and novel artificial 2D lattices.



**Fig.1** Chemical vapour deposition of 2D transition metal dichalcogenides

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**Dr. Yumeng Shi** is Professor of International Collaborative Laboratory of 2D Materials for Optoelectronics Science and Technology (2D MOST) of Shenzhen University, China.



His current research interests include synthesis of 2D materials and their applications in optoelectronics. Prof. Shi's research experience is highly interdisciplinary. He has been exposed to various fields of materials science and engineering including organic and inorganic semiconducting electronics (OPV, OLED and FETs), sensors (Gas-sensing, Bio-sensing and Photo-sensing), and chemical vapor deposition (for graphene, h-BN and MoS<sub>2</sub>). He has obtained 1 USA patent and published more than 70 research papers in prestigious academic journals including Science, Chem Soc Rev, Advanced Materials, Nano Today, Nano Letters, ACS Nano, Physics Review Letters, Small, Journal of Materials Chemistry, Physical Review B and et al. with a total citation >7000, H-Index 30.

For more information, please visit <http://yumengshi.wix.com/optoelectronics>.



**Session B1****B02****8:25 - 8:50 AM Room B June 20****Hysteresis of Transfer Characteristics in Field-Effect Transistors with a Molybdenum Disulfide Channel**

Yoshihiro Shimazu

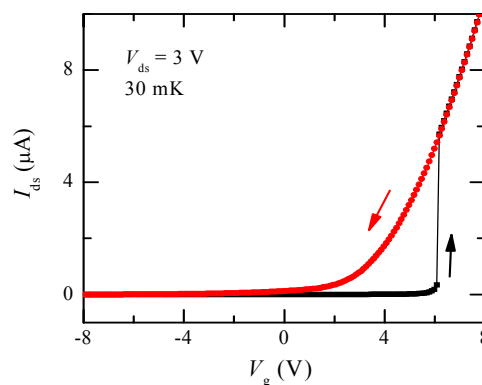
Department of Physics, Yokohama National University

79-5, Hodogaya, Yokohama 240-8501, Japan

Email: yshimazu@ynu.ac.jp

**Abstract**

Recent studies on single- and multilayer molybdenum disulfide ( $\text{MoS}_2$ ) devices have revealed their promising characteristics as novel semiconductor devices. Here, we report the effects of environmental gases on the hysteresis in the transfer characteristics and observation of an anomalously large hysteresis below 1K for back-gated multilayered  $\text{MoS}_2$  field-effect transistors [1,2]. Comparisons between different gases (oxygen, nitrogen, air, and nitrogen with varying relative humidities) revealed that water molecules acting as charge-trapping (dominantly hole-trapping) centers are the main cause of hysteresis. While the hysteresis persisted even after pumping out the environmental gas for longer than 24 h at room temperature, it disappeared when the device was cooled to 240 K, suggesting a considerable increase in the time constant of the charge trapping/detrapping at these modestly low temperatures. Below 1 K, we observed for the first time an anomalously large hysteresis, which is not attributed to charge trapping. We hypothesize that this hysteresis results from the slow injection of electrons via quantum tunneling through the Schottky barrier at the contacts. The size of the hysteresis increased with increase in the scan rate of the gate voltage, which is consistent with the possibility of very slow injection of electrons.



**Fig.1** Transfer characteristics of a back-gated  $\text{MoS}_2$  FET with Cr/Au contacts measured at 30 mK. The thickness of the  $\text{MoS}_2$  flake is  $\sim 70$  nm. A large hysteresis with an abrupt jump in the drain-source current is observed.

**References**

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**Yoshihiro Shimazu** is Associate Professor in Department of Physics of Yokohama National University since 1996. He received his Ph. D. in physics in 1993 from the University of Tokyo. He is a Member of the Physical Society of Japan.



In 1991-1996, he studied experimental solid state physics at the University of Tokyo, using low-temperature environments (including dilution refrigerators) and microfabrication technique. In 1999-2000, he worked as a visiting scientist at Delft University of Technology, where he experimentally studied a superconducting quantum bit based on small Josephson junctions.

His current research interests include electric-field effects and low-temperature transport in 2D materials (transition-metal dichalcogenides, transition-metal monochalcogenides, misfit layer compounds, graphene etc.), and micro/nano fabrication of electronic devices, novel superconducting materials, and quantum phenomena in mesoscopic systems.

**Session B1**

**B03**

**8:50 - 9:15 AM Room B June 20**

## Valley Edelstein Effect in Monolayer Transition Metal Dichalcogenides

\*KATSUHISA TAGUCHI, YUKI KAWAGUCHI, YUKIO TANAKA

Department of Applied Physics, Nagoya University, Nagoya, 464-8603, Japan

Email: \*taguchi@rover.nuap.nagoya-u.ac.jp

KAM TUEN LAW

Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China

### Abstract

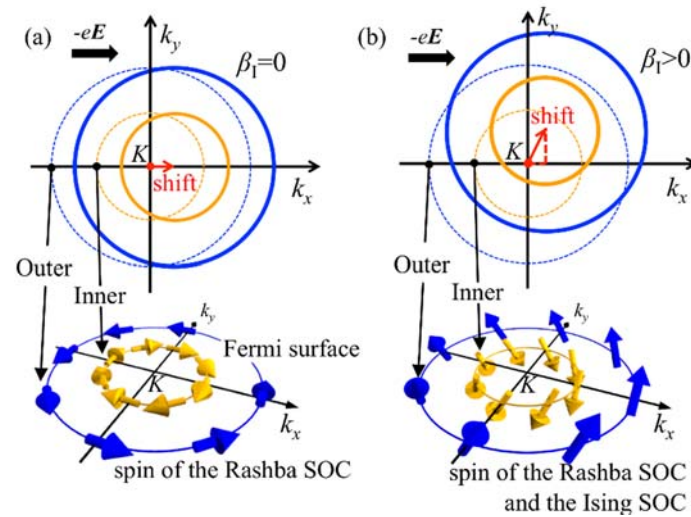
Monolayer transition metal dichalcogenides (MTMDs) exhibit spin-orbit coupling (SOC) called Ising SOC, which polarizes electron spins to opposite out-of-plane directions for electrons in opposite valleys. So far, several valley-dependent phenomena, such as valley-selective circularly dichroism [1] and valley-Hall effect [2], have been theoretically studied and experimentally reported. These valley-dependent phenomena have applications for electronics and optics using valley-degrees of freedom. Here, we theoretically predict the valley Edelstein Effect (VEE), which is an electric-field-induced spin polarization effect, in the MTMDs in the presence of Rashba and Ising SOC [3]. The spin polarization due to the VEE is given by

$$\langle \mathbf{s}_v^{\text{VEE}} \rangle = e\nu_e [\mathcal{C}_\perp (\hat{\mathbf{z}} \times \mathbf{E}) + v\mathcal{C}_\parallel \mathbf{E}]$$

where  $v=\pm 1$  is the index denoting the valley degrees of freedom,  $e$  is the elementary charge of an electron,  $\nu_e$  is the 2D density of states with  $m$  being the effective electron mass,  $\mathbf{z}$  is a unit vector normal to the system, and  $\mathcal{C}_\perp$  and  $\mathcal{C}_\parallel$  are the response coefficients that we calculate in the following sections.

The second term in the above equation is the main result in this work.

We found an unconventional valley-dependent response in which the spin-polarization is parallel to the applied electric field and the spin-polarization is opposite at opposite valleys due to the Ising SOC. This is in sharp contrast to usual Edelstein effect in which the induced spin-polarization is perpendicular to the applied electric field. We attribute the VEE to the valley Hall effect and Ising SOC [See Fig.1]. Since the conventional Edelstein effect is promising to spintronics devices, our obtained VEE can be useful for an application to electronics devices with spin and valley-degrees of freedom.



**Fig.1** Mechanism for (a) the conventional Edelstein effect at  $\beta_1=0$  and (b) the VEE at  $\beta_1 \neq 0$ . The top panels show the shift of the Fermi surface around the  $K$  point, where the dashed (solid) lines represent the spin-split Fermi surfaces in the absence (presence) of an applied electric field. The spin structures on the Fermi surface are depicted in the bottom panels. Due to the Ising SOC, the spins have the longitudinal component, which shifts the Fermi surfaces perpendicular to the applied field via the valley Hall effect as shown in (b).

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**Katsuhisa Taguchi (PD).** Current research interests include transport in the field of spintronics and topological materials.



Session B1

B04

9:15 - 9:40 AM Room B June 20

## Growth of TMDC Nanostructures by Chemical Vapor Deposition

TOSHIHIRO SHIMADA, MENGTING WENG, TAKASHI YANASE, SHO WATANABE, FUMIYA UEHARA,  
TARO NAGAHAMA

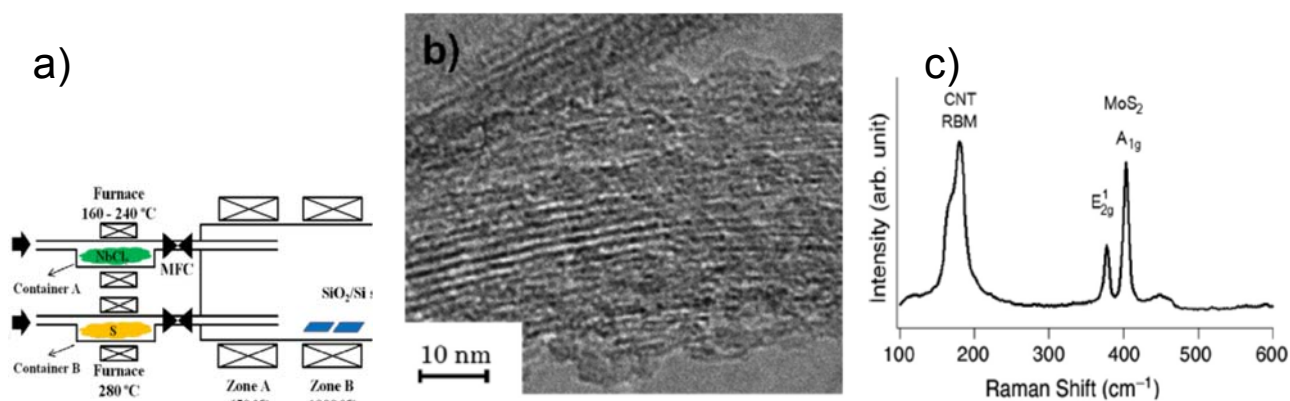
Division of Applied Chemistry, Hokkaido University

Kita-ku, Sapporo 060-8628, Hokkaido

Email: shimadat@eng.hokudai.ac.jp

### Abstract

Chemical vapor deposition (CVD) is a simple but powerful technique to synthesize thin films of various materials. It can also be used to synthesize nano-structured materials if it is used with nano-structured templates or catalysts. We have developed separate flow CVD system to make multilayered transition metal dichalcogenides (TMDCs) or doped layers [1,2]. We used the apparatus to make nanocomposite between carbon nanotube and MoS<sub>2</sub> that was applied to photovoltaic applications (Fig.1) [3]. We also describe the search for the catalysts to make TMDC nanostructures.



**Fig.1** (a) Separate flow CVD[1,2] (b) TEM image and (c) Raman spectrum of MoS<sub>2</sub> nano flakes grown on carbon nanotube bundles[3].

## **References**

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Jeon et al., *Org. Electron.* 17, 285 (2015).



**Toshihiro Shimada** is Professor of Applied Chemistry and Division Chair. He is a Member of Chemical Society of Japan, Japan Society of Applied Chemistry, Japanese Ceramics Society, Japanese Electric Society. He is an editorial board member of *Chemistry Letters*.

His current research interests include materials synthesis and functions of nanostructured materials, carbon, atomic layer materials, organic semiconductors.



For more information, please visit  
<http://www.eng.hokudai.ac.jp/labo/kotai/index.html>

**Session B1**

**B05**

**9:40 - 10:05 AM Room B June 20**

## Electrocatalytic hydrogen evolution reaction of MX<sub>2</sub> and MX<sub>2</sub> heterostructures

YANFENG ZHANG

Department of Materials Science and Engineering, College of Engineering

Peking University, Beijing 100871, P. R. China

Email: yanfengzhang@pku.edu.cn

### Abstract

Advanced materials for electrocatalytic and photoelectrochemical water splitting are central to the area of renewable energy. Recently, two dimensional layered materials of MX<sub>2</sub> (M: Mo, W; X: S, Se, etc.) have emerged as a new kind of catalysts for such applications. Our group have reported the direct synthesis of high-quality, domain size tunable, strictly monolayer MoS<sub>2</sub> flakes on commercially available Au foils by a chemical vapor deposition (CVD) method. The nano-sized triangular MoS<sub>2</sub> flakes on Au foils are proven to be excellent electrocatalysts for hydrogen evolution reaction (HER), featured by a rather low Tafel slope (61 mV/dec) and a relative high exchange current density (38.1 μA/cm<sup>2</sup>). The excellent electron coupling between MoS<sub>2</sub> and Au foils is considered to account for the extraordinary HER activity [1]. Furthermore, via a facile all-CVD approach, we have also demonstrated the direct growth of monolayer MoS<sub>2</sub> on graphene (MoS<sub>2</sub>/Gr) over Au foils [2, 3]. A dramatic decrease of the bandgap from ~2.20 to ~0.30 eV was detected at the domain edge of MoS<sub>2</sub> within a lateral distance of ~6 nm, as evidenced by STM/STS observations. The edges of monolayer MoS<sub>2</sub> nano-sheets were thus served as narrow-gap quantum wires, which can greatly facilitate the electrocatalytic property of MoS<sub>2</sub> in HER [4]. Meanwhile, we also synthesized either MoS<sub>2</sub>/WS<sub>2</sub> or WS<sub>2</sub>/MoS<sub>2</sub> vertical heterostructures on Au foils by a growth-temperature-mediated, selective two-step CVD strategy. Relative enhancement or reduction in the photocatalytic activities were observed for MoS<sub>2</sub>/WS<sub>2</sub> and WS<sub>2</sub>/MoS<sub>2</sub> in HER under illumination, respectively. This is explained from the type-II band alignment of the MoS<sub>2</sub>/WS<sub>2</sub> stack that enables effective electron-hole separation and fast electron transfer kinetics, as well as directional electron flow from electrode to catalytically active sites [5]. The abovementioned efforts are expected to establish the internal relationship between the metallic edge states of MoS<sub>2</sub> and its HER performances, as well as the advantage of MX<sub>2</sub>/MX<sub>2</sub> vertical stacks in photocatalytic HER applications.

**Keywords:** MX<sub>2</sub>, Heterostructures, Hydrogen evolution reaction.

## **References**

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**Yanfeng Zhang** is a Professor of College of Engineering of Peking University, and the Center for Nanochemistry of Peking University. She has been offered several prizes and honors, including 100 National Excellent Doctoral Dissertation (2006), Peking University 100 Talent Program (2010), National Science Fund for Distinguished Young Scholars of China (2012), and Young Scholars of the Yangtze River (2016).



Her current research interests include the controlled growth, accurate characterization and novel property exploration of two dimensional layered materials including graphene, h-BN-graphene heterostructures, and transition metal dichalcogenides (TMDCs) and their heterostructures. She has published more than 110 papers on international journals, including *Science*, *Nature Commun.*, *Phys. Rev. Lett.*, *J. Am. Chem. Soc.*, *Nano Lett.*, *Adv. Mater.*, etc.

For more information, please visit <http://www.chem.pku.edu.cn/cnc/cn/zxcy/jy/253325.shtml>.

**Session B2**

**B06**

**10:20 - 10:45 AM Room B June 20**

## Prelithiated Si nanoparticles-carbon nanotubes composite anodes for Li-ion batteries

KANG YAO<sup>(a)(b)(c)</sup>, RICHARD LIANG<sup>(a)(c)(f)</sup>, and JIM P. ZHENG<sup>(a)(b)(d)(e)</sup>

<sup>(a)</sup>Materials Science & Engineering,

<sup>(b)</sup>Aero-propulsion, Mechatronics and Energy Center,

<sup>(c)</sup>High-Performance Materials Institute,

<sup>(d)</sup>Center for Advanced Power Systems, Florida State University;

<sup>(e)</sup>Department of Electrical & Computer Engineering

<sup>(f)</sup>Department of Industrial and Manufacturing Engineering

Florida A&M University-Florida State University, Tallahassee, FL 32310, USA

Email: zheng@eng.famu.fsu.edu

### Abstract

Freestanding flexible Si nanoparticles-multi-walled carbon nanotubes (SiNPs-MWNTs) composite paper anodes for Li-ion batteries (LIBs) have been prepared using a combination of ultra-sonication and pressure filtration. No conductive additive, binder or metal current collector is used. The SiNPs-MWNTs composite electrode material achieves first cycle specific discharge and charge capacities of 2298 and 1492 mAh/g, respectively. To address the first cycle irreversibility, stabilized Li metal powder (SLMP) has been utilized to pre-lithiate the composite anodes. As a result, the first cycle irreversible capacity loss is reduced from 806 to 28 mAh/g and the first cycle coulombic efficiency is increased from 65% to 98%. The relationship between different SLMP loadings and cell performance has been established to understand the pre-lithiation process of SLMP and to optimize the construction of Si-based cells. A cell containing the pre-lithiated anode is able to deliver charge capacity over 800 mAh/g without undergoing the initial discharge process, which enables the exploration of novel cathode materials.

It was also found out the SiNPs-MWNTs electrode with 3:2 Si/MWNT ratio exhibits the optimal balance between the high capacity of SiNPs and the high electrical conductivity and structural stabilization quality of MWNTs, leading to a high rate capability, high specific capacity, and cycle life surpassing the conventional slurry-cast SiNPs electrode using binder and Cu current collector. The reversible capacity is 1866 mAh/g (based on the total composite weight, the same below) at current density of 100 mA/g. After 100 cycles, the electrode retains capacity of 1170 mAh/g at 100 mA/g and 750 mAh/g at 500 mA/g. The superior performance is believed to be due to the cooperative or even synergistic effect achieved by the optimal combination. Furthermore, the freestanding feature of our electrode eliminates the non-active mass, which is promising for enhanced capacity and energy density of Li-ion cells.

**Dr. Jim P. Zheng** is a Sprint Eminent Scholar Chair Professor at the Department of Electrical and Computer Engineering of Florida A&M University (FAMU) and Florida State University (FSU). He is the recipient of National Academy of Inventors Fellow, National Research Council Fellow, Army Research & Development Achievement Award, NASA Faculty Research Award, and Progress Energy Professional Development Award. He has published more than 120 articles in scholarly journals, and 110 papers in conference proceedings in the fields of energy storage, fuel cells, nano-sensors, photonics, and thin film growth, and been awarded 18 patents. He is the founder of General Capacitor LLC and a co-founder of Bing Energy International Inc. He serves as editorial board of the Journal of Materials. Zheng is a senior member of the Institute of Electrical and Electronic Engineers and member of the Electrochemical Society.



Phone: (850) 410-6464, Email: [zheng@eng.fsu.edu](mailto:zheng@eng.fsu.edu)

**Session B2**

**B07**

**10:45 - 11:10 AM Room B June 20**

## Investigating structure and stress evolution in Si anode using *in situ* high pressure technique and Raman microscopy

ZHIDAN ZENG

Center for High Pressure Science and Technology Advanced Research (HPSTAR)

Bldg 6, 1690 Cailun Road, Shanghai 201203, China

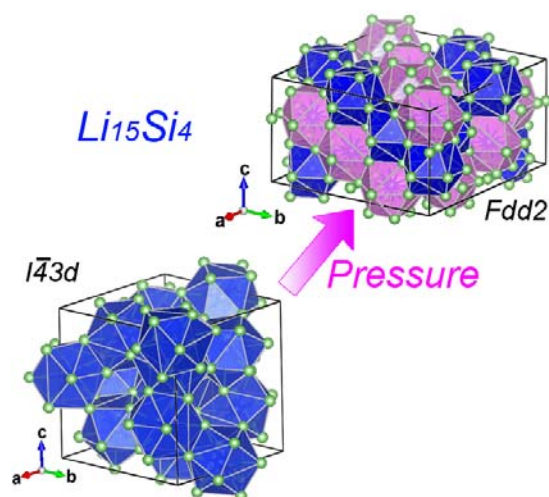
Email: zengzd@hpstar.ac.cn

### Abstract

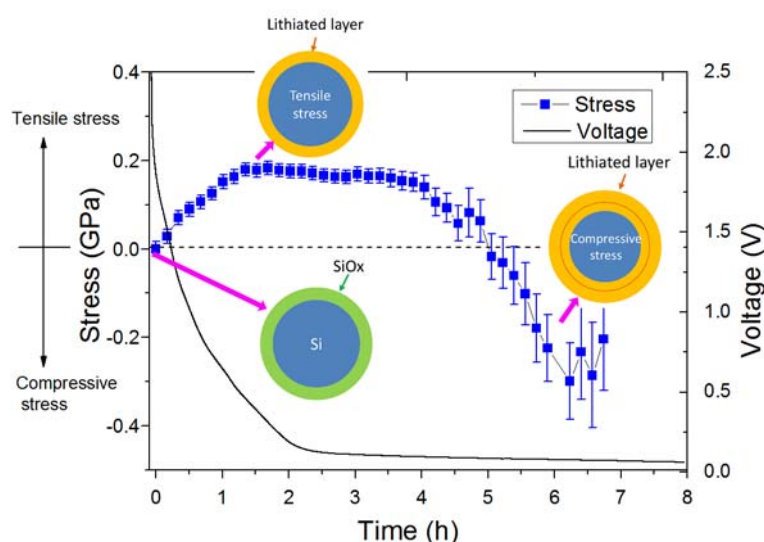
Silicon is widely regarded as one of the most promising anode materials for next-generation lithium-ion batteries, making Li-Si an important energy storage system. During Li insertion into Si, stress of gigapascal level is introduced accompanied by a volume expansion up to 280%, alters properties of materials, and leads to mechanical failure of Si anodes.

$\text{Li}_{15}\text{Si}_4$  (alpha-  $\text{Li}_{15}\text{Si}_4$ , space group: I-43d), the only crystalline phase that forms during lithiation of the Si anode in lithium-ion batteries, was found to undergo a structural transition to a new phase (beta-  $\text{Li}_{15}\text{Si}_4$ ) at approximately 7 GPa (see Fig.1). *Ab initio* evolutionary metadynamics calculations suggest beta-  $\text{Li}_{15}\text{Si}_4$  has an orthorhombic structure with an Fdd2 space group. This new beta-  $\text{Li}_{15}\text{Si}_4$  has substantially larger elastic moduli compared with alpha-  $\text{Li}_{15}\text{Si}_4$ , and has good electrical conductivity. As a result, beta-  $\text{Li}_{15}\text{Si}_4$  has superior resistance to deformation and fracture under stress. The theoretical volume expansion of Si would decrease 25% if it transformed to beta-  $\text{Li}_{15}\text{Si}_4$ , instead of alpha-  $\text{Li}_{15}\text{Si}_4$ , during lithiation. In addition, the fact that beta-  $\text{Li}_{15}\text{Si}_4$  can be recovered back to ambient pressure, provides opportunities to further investigate its properties and potential applications. [1]

Nanostructured Si are important materials to address mechanical stress issues in batteries although their stress were only calculated and no experimental data are available. Using *in situ* Raman microscopy to monitor the shift of the first-order Raman peak of Si, we were able to measure for the first time the lithiation-induced stress in Si nanoparticles. The shift of Raman peak of Si under hydrostatic stress was calibrated via an *in situ* high pressure Raman experiment. We observed a transition in the stress in Si core of nanoparticles during lithiation, from tensile to compressive (see Fig.2). At the beginning of lithiation, the reduction of the native oxide surface layer of the Si particle results in a tensile stress of approximately 0.2 GPa in Si. During the formation of amorphous  $\text{Li}_x\text{Si}$  in the outer layer of the nanoparticles, an increasing compressive stress up to 0.3 GPa is introduced to the Si core. This evolving stress explains the cracks that developed in the amorphous  $\text{Li}_x\text{Si}$  layer during lithiation of the Si nanoparticles, and is also consistent with modeling results. These results improve our understanding of lithiation-induced stress in nanostructured Si anodes, and provide valuable information for their theoretical study and future design. [2]



**Fig.1** The atomic structure of alpha-Li<sub>15</sub>Si<sub>4</sub> (lower left) and beta-Li<sub>15</sub>Si<sub>4</sub> (upper right). Each silicon atom is surrounded by lithium atoms (green spheres) with the coordination number of 12 (shown in blue polyhedra) or 13 (shown in pink polyhedra)



**Fig.2** The stress in Si nanoparticles (left y-axis) and the potential of the half cell versus Li<sup>+</sup>/Li (right y-axis) as a function of lithiation duration.

## References

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**Zhidan Zeng** is Staff Scientist in Center for High Pressure Science & Technology Advanced Research. Her research interests are using various high pressure techniques to understand the structure and properties of energy-related materials and group-14 elements (carbon, silicon, germanium, and related materials) under extreme conditions; synthesis of novel super-hard materials; mechanical properties and deformation of materials.



**Session B2**

**B08**

**11:10 - 11:35 AM Room B June 20**

## Silicon-based anode materials for high capacity lithium ion batteries

JUNYING ZHANG AND CHUANBO LI\*

State Key Laboratory on Integrated Optoelectronics, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China

Email: \*cbli@semi.ac.cn

### Abstract

Developing an anode material with high-energy capacity is crucial to improve the performance of rechargeable batteries. Si is an important anode candidate because of its large lithium storage capacity ( $4200 \text{ mAhg}^{-1}$ , about 10 times higher than graphite), ( $372 \text{ mAhg}^{-1}$ ), low lithium alloying/dealloying potential, long discharge plateau, and abundance. However, the huge volume expansion/shrinkage of Si particles during charge/discharge cycles results in the pulverization of electrode structure and causes considerable capacity decay. The lack of electronic contacts between Si particles or between active coating materials and current collectors reduces its capacity. Many investigations have been carried out to accommodate this severe volume expansion including novel nanostructured Si, such as Si wires, Si tubes, porous thin films, and nest-like Si nanospheres, and multiphase composites with active Si and other active/inactive phases. However, the nano-sized Si particles would agglomerate during cycling which will decrease the cycling performance, due to high electrochemical activity. In this presentation, micro-sized polycrystalline Si particles have reduced agglomeration effect compared to nano-sized ones. We find that the electrochemical performances can be improved greatly by introducing proper binder to protect the electrode from cracking and using suitable conductive agent to provide an efficient conductive channel. By introducing nano-porous structures through chemical etching, the huge volume expansion can be effectively relieved by maintaining the complete structure of Si particles during charge/discharge cycles. Moreover, combined with carbon coating which is attractive owing to the conductive and ductile features of carbon, the conductivity can be improved and the volume expansion/shrinkage of Si can be further decreased. Developing nano-porous structure combining with pyrolyzed polyacrylonitrile could form a novel composite electrode. The electrochemical performance can be considerably improved with a conductive carbon network and nano-porous structure together with carbon layer accommodate the volume expansion/shrinkage during charge/discharge cycles.

**Chuanbo Li** is the professor of Institute of Semiconductors, Chinese Academy of Sciences. He gets the support of 1000 talent program for young scientists and his research interests include Si based materials for optoelectronic devices and lithium battery. He has 7 years research experience in Imperial College London and Tokyo Institute of Technology. He has published over 100 papers and holds 7 patents. He was committee of several international conference like IEEE GFP 2016, 2017 and ECS PRiME 2018 (G05) and so on.



**Session B2**

**B09**

**11:35 - 12:00 PM Room B June 20**

## Efficient Solar-Rechargeable Lithium Ion Battery Energy Storage

QIQUAN QIAO

Center for Advanced Photovoltaics, Electrical Engineering and Computer Science Department, South Dakota State University, Brookings, SD 57007, USA

Email: Qiquan.Qiao@sdstate.edu

### **Abstract**

Use of energy storage devices such as lithium ion batteries (LIBs) can help to mitigate the problem of intermittent photovoltaic (PV) power to achieve higher PV penetration into the electric grid. Also, the benefit of deployment of electric vehicles for energy sustainable future seems rather irrelevant unless they are charged using electricity generated from renewables. In addition, large scale practical applications of battery based electric vehicles is still challenging because of the inflexibility it has with the charging stations. All these issues can be addressed by use of solar cells as a viable energy source to charge lithium ion batteries. Here we demonstrate simple, efficient and cost effective photo-charging design approach where the use of promising low cost solar cells such as perovskite solar cell or dye sensitized solar cell with the help of DC-DC power conversion can efficiently charge a  $\text{Li}_4\text{Ti}_5\text{O}_{12}\text{-LiCoO}_2$  LIB.

**Dr. Qiquan Qiao** is Harold C. Hohbach Professor and graduate coordinator in Electrical Engineering at South Dakota State University (SDSU). Current research focuses on polymer photovoltaics, dye-sensitized solar cells, Perovskite solar cells, lithium ion batteries, biosensors and agriculture sensors. He has published more than 100 peer reviewed papers in leading journals including Energy and Environmental Science, Journal of the American Chemical Society, Advanced Materials, Advanced Energy Materials, Advanced Functional Materials, Nanoscale, and Nano Energy, etc. He has received more than \$6.5 million research grants as PI or Co-PI. He has 2015 Distinguished Researcher Award from SDSU, received 2014 F O Butler Award for Excellence in Research at SDSU, 2010 US NSF CAREER, and 2009 Bergmann Memorial Award from the US-Israel Bi-national Science Foundation.



Session B3

B10

14:00 - 14:25 PM Room B June 20

## High performances flexible energy storage devices

BIN WANG

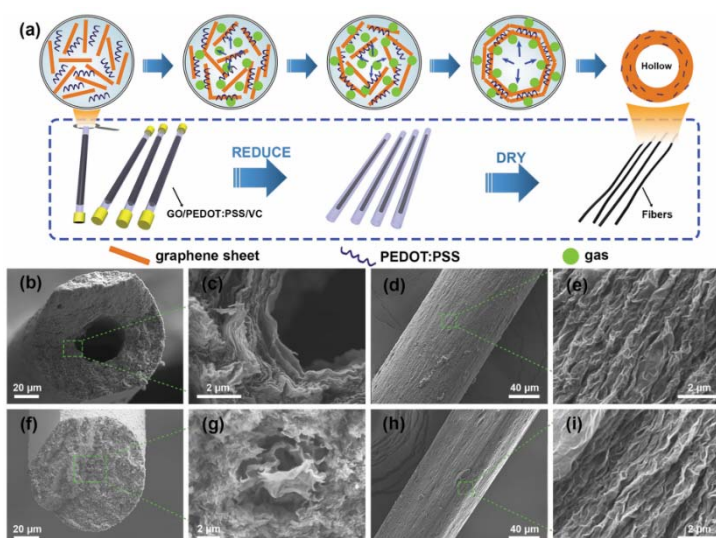
Institute of Chemical Materials,China Academy of Engineering Physics

No.596 Yinhe Road, Chengdu, Sichuan, China

Email: binwang@caep.cn, edward.bwang@gmail.com

### Abstract

In this work, the flexible fiber-shaped supercapacitors have been fabricated by using the conductive polymers and graphene as the electrodes. The prepared fiber-shaped electrodes show good mechanical properties and excellent electrochemical performances. They can be easily knotted, twisted and woven into different shapes without sacrificing their electrochemical properties. [1-2].



*Fig.1 Schematic illustration and the SEM images of HCFs and formation of hollow structures.*

### References

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- [2] B.Wang et al, Functionalized carbon nanotubes and graphene-based materials for energy storage, *Chem.Comm.*,2016, 52, 14350.

**Bin Wang** is a Principal Investigator of National Energy Novel Materials Center and China academy of engineering physics (CAEP). He obtained his Ph.D degree from Fudan University in 2009, and then he worked as a postdoc fellow at LBNL, USA. In 2013, he went back to China and worked at Institute of Chemical Materials, CAEP as a staff scientist. He is selected as Expert Fellow of China Energy Society, the National 1000plan youth talent and awarded as the Membership Award of American Chemical Society, Excellent contribution honor in 17th IUPAC NMS. He has published more than 60 professional papers; including 5 ESI highly cited papers and several cover/back cover papers. The time cited: >2200, h-index:26, i10-index:43.



His current research interests include flexible energy conversion and storage devices, high safety lithium-ion battery and gas sensor.

For more information, please visit <http://scholar.google.com/citations?user=qPQY9YcAAAAJ>.

**Session B3**

**B11**

**14:25 - 14:50 PM Room B June 20**

## **Porous carbon fibers for electromagnetic wave absorption**

CHUN SHAN, LINCHANG MAO, KANG FU, GUANG LI\*

State key laboratory for modification of chemical fibers and polymer materials, Donghua University,

Email: lig@dhu.edu.cn

### **Abstract**

Modern warfare urgently needs radar stealth technology to meet the shelter requirements of weapons and equipment. In this paper, porous carbon fibers were developed as an efficient microwave absorbent filler to prepare microwave absorbing composites. Firstly, polyacrylonitrile (PAN) was used as carbon precursor polymer (CPP), while polymethyl methacrylate (PMMA) as thermally decomposed polymer (TDP). PAN/PMMA (70/30) blend fibers were prepared by a wet spinning of PAN/PMMA solutions. Secondly, Porous carbon fibers (PCF) were obtained through carbonization of the blend fibers. The molecular weight of PAN could be used to control the size of pores in PCF, that is, when the average molecular weight of PAN was 51,000 g/mol and 83,000 g/mol respectively, PCF with pores ranging 1-10 $\mu$ m in diameter (designated PCF-L); and the other one with pores with diameter in the range of 0.1-1  $\mu$ m (designated PCF-S) were obtained. The resultant porous fibers, PCF-L and PCF-S, were used as microwave absorbing fillers to mix with epoxy respectively, the composites containing 2-6 wt% of the filler were fabricated. It was found that PCF-S filled composites showed much better microwave absorption performance than that PCF-L filled one. The composite containing 6 wt% of PCF-S reached the lowest reflection loss of -32dB; and the reflection loss below -10 dB covered the whole X band. The change or destruction of the porous structure in PCF showed great effect on the microwave absorption properties, which demonstrate that the pores in PCF could make great contribution to the microwave absorption.

**Keywords:** Porous carbon fibers; microwave absorbent; composites; reflection loss; microwave absorbing mechanism



**Dr. Guang Li** is a Professor, Ph.D Supervisor in the College of Material Science and Engineering at Donghua University (China). Dr. Li received her M.Sc in Chemistry from China Textile University in 1985, and her Ph.D in material science and engineering from Donghua University in 2006, respectively. Dr. Li was as an Assistant Professor, a Lecturer then an Associate Professor at China Textile University from 1986 to 1999. She was a Senior Visiting Scholar in the University of Twente (Netherlands). Dr. Li was promoted to be a full Professor at Donghua University (China) in 1999, and is continuously working on high performance polymer synthesis, porous carbon fibers and their associated processing for energy applications including PEM fuel cells. Dr. Li has led more than 20 projects supported by Chinese National Natural Science Foundation, Ministry of Education of China, Shanghai Municipal Science and Technology Commission, etc. Dr. Li has published more than 100 scientific papers in high-impacting peer-reviewed journals. She has given more than 24 invited/oral presentations in international conferences, co-authored 4 books, and owns 26 patents. Dr. Li has been awarded several prizes for recognizing her great contributions to science and technology, including the second prize of science and technology progress in Shanghai, the second prize from Ministry of education of China, the second prize from China textile industry association, etc.



**Session B3**

**B12**

**14:50 - 15:15 PM Room B June 20**

## High Temperature Flexible Supercapacitors Using Graphene Electrodes

HO SEOK PARK

Affiliation (Company / Institution)

School of Chemical Engineering & Samsung Advanced Institute for Health Science & Technology (SAIHST),

Sungkyunkwan University (SKKU), Suwon 440-746, Republic of Korea

Email: phs0727@skku.edu

### Abstract

With increasing demand for high performance energy storage systems, the feasibility of reliable and functional energy storage devices that well operates under extreme conditions is of prime importance for expanding applicative fields as well as for understanding materials' intrinsic and extrinsic properties and device physics. Our group has been investigating the control in the physical structure and chemical composition of 2D graphenes and beyond for ultracapacitive energy storage devices under limited circumstances, where conditions are classified into thermodynamic (e.g. pressure, volume and temperature) and kinetic (e.g. high rate and frequency) variables. We also studied a fundamental foundation *via in-situ* spectroscopic techniques to understand charge storage phenomenon of new materials and devices occurring on a nanoscale under various circumstances. In this talk, I will introduce high temperature operating, flexible supercapacitors based on graphene electrodes that can efficiently deliver electrical energy under electrochemical, mechanical and thermal stresses.[1-4] In order to achieve high performance supercapacitor devices under thermal, mechanical and electrochemical stresses, the micro- and macroscopic structures and chemical compositions of graphenes are delicately controlled by chemical modification. A new generation of flexible supercapacitors, with the long-term durability and outstanding electrochemical properties, were realized, showing a high position of the Ragone plot, even under severe conditions.

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**Ho Seok Park** is an associate professor at the School of Chemical Engineering of Sungkyunkwan University (SKKU). He is a concurrent professor at the Samsung Advanced Institute of Health Science & Technology (SAIHST) of SKKU. He is an editorial member of SCI(E) journals titled by “Macromolecular Research” and “Carbon Letters”. He published ~ 110 papers including top journals such as Nano Lett., ACS Nano, JACS, EES, Adv. Mater., Adv. Energy Mater., Adv. Funct. Mater. and Nano Energy.



His current research interests include the nanostructured materials for applications into electrochemical energy conversion and storage as well as porous carbon nanomaterials for applications into CO<sub>2</sub> capture and conversion and water purification.

For more information, please visit <http://esem.skku.edu>.

## Session B3

## B13

15:15 - 15:40 PM Room B June 20

## Rational Design of Novel Carbon Catalysts for Clean Energy Conversion and Storage

ZHENGHANG ZHAO, ZHENHAI XIA

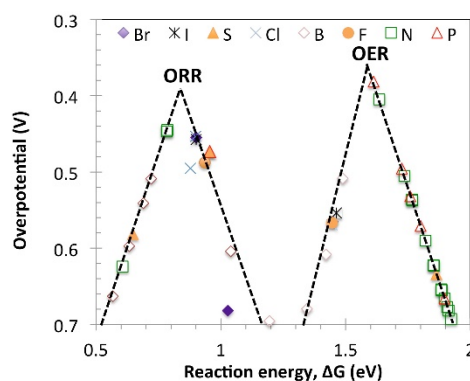
University of North Texas

3940 North Elm St., Denton, TX 76203, USA

Email: zhenhai.xia@unt.edu

**Abstract**

In fuel cells and metal-air batteries, there are critical chemical reactions: *oxygen reduction reaction* (ORR), and *oxygen evolution reaction* (OER), respectively. These reactions, however, are sluggish and require noble metals (*e.g.*, platinum) or their oxides as catalysts. The scarcity and high cost of noble metals have hampered the commercial applications of these technologies.[1] Therefore, it is necessary to search for alternative materials to replace Pt. Carbon nanomaterials, such as carbon nanotubes (CNTs) and graphene, are appealing as an alternative for metal-free catalytic applications because of their structures and excellent properties. Although the superior catalytic capabilities of heteroatom-doped carbon nanomaterials for ORR have been demonstrated, trial-and-error approaches are still used to date for the development of highly-efficient catalysts. To rationally design a catalyst, it is critical to correlate intrinsic material characteristics with catalytic activities. Through first-principles calculations, we have identified a material property that serves as the activity descriptor for both ORR and OER, and established a volcano relationship between the descriptor and the catalytic activities of the carbon-based nanomaterials.[2] The design principles can be used as a guidance to develop various new carbon-based materials for clean energy conversion and storage.



**Fig.1** Volcano relationships between the descriptor and the catalytic activities of the carbon-based nanomaterials

## **References**

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**Zhenhai Xia** is Professor of Department of Materials Science and Engineering, Department of Chemistry at University of North Texas, USA. He is a Member of American Society of Mechanical engineers, and Materials Research Society, He was the recipient of German Humboldt Scholar Award in 1997, and “Nanoscience Research Leader Award” from Science Letters in 2015, and Changjiang Scholar Award from China Ministry of Education in 2016.



His current research interests include energy conversion and storage, bioinspired materials, and multiscale modeling and simulation.

For more information, please visit <http://www.mtse.unt.edu/XiaGroup/>

**Session B4**

**B14**

**16:00 - 16:25 PM Room B June 20**

## Kilohertz supercapacitors based on graphene and carbon fiber for AC filtering and energy harvesting

ZHAOYANG FAN

Department of Electrical and Computer Engineering and Nano Tech Center,  
Texas Tech University, Lubbock, TX 79409, USA

Email: Zhaoyang.Fan@ttu.edu

### **Abstract**

High-frequency supercapacitors are being studied with the aim to replace the bulky electrolytic capacitors for current ripple filtering and other functions used in power systems. Here 3D edge-oriented graphene (EOG) was grown encircling carbon nanofiber (CNF) framework to form highly conductive electrode with a large surface area. Such EOG/CNF electrodes were tested in aqueous and organic electrolytes for high-frequency supercapacitor development. For the aqueous cell and the organic cell, the characteristic frequency at  $-45^\circ$  phase angle was found to be as high as 22 kHz and 8.5 kHz, respectively. At 120 Hz, the electrode capacitance density was  $0.37 \text{ mF cm}^{-2}$  and  $0.16 \text{ mF cm}^{-2}$  for the two cells. In particular, the 3V high-frequency organic cell was successfully tested as filtering capacitor used in AC/DC converter, suggesting the promising potential of this technology for compact power supply design and other applications.

**Zhaoyang Fan** is Professor of Electrical and Computer Engineering at Texas Tech University. He is a Senior Member of IEEE and a Member of APS and MRS. He is a recipient of Whitacre Engineering Research Award and also a Senior Member of TTU System Chapter of National Academy of Inventors.

His current research interests include thin-films and nanomaterials for photonics, photovoltaics, energy conversion and storage.

For more information, please visit <http://myweb.ttu.edu/zfan/index.html>





**Session B4**

**B15**

**16:25 - 16:50 PM Room B June 20**

**Composite AgBr colloidal spheres/g-C<sub>3</sub>N<sub>4</sub> nanosheets: An effective LED-irradiation photocatalyst**

GUOCHANG CHEN<sup>a\*</sup>, CUN-YUE GUO<sup>b</sup>, MINGFU YE<sup>a</sup>, HONGBIN QIAO<sup>a</sup>, LIXIN XU<sup>a</sup>, XIANWEN WEI<sup>a\*</sup>

<sup>a</sup> College of Chemistry and Chemical Engineering

Anhui University of Technology, Ma'anshan 243002, P. R. China

<sup>b</sup> School of Chemistry and Chemical Engineering

University of Chinese Academy of Sciences, Beijing 100049, P. R. China

Email: chenguochang@iccas.ac.cn (G. Chen). xwwei@mail.ahnu.edu.cn (X. Wei)

**Abstract**

The g-C<sub>3</sub>N<sub>4</sub> nanosheets were fabricated with guanidine hydrochloride and NH<sub>4</sub>Cl as the precursor and AgBr colloidal spheres were uniformly dispersed on the curly g-C<sub>3</sub>N<sub>4</sub> ultrathin nanosheets to form the composite AgBr/g-C<sub>3</sub>N<sub>4</sub>. The introduction of g-C<sub>3</sub>N<sub>4</sub> improved the stability of AgBr and optimized spatial charge carrier transfer. The as-prepared AgBr/g-C<sub>3</sub>N<sub>4</sub> afforded excellent activities toward methyl orange (MO) degradation under the LED-irradiation. The separation mechanism of photoexcited carriers for the photocatalyst was accordingly proposed.

**Keywords:** AgBr/g-C<sub>3</sub>N<sub>4</sub>; AgBr; g-C<sub>3</sub>N<sub>4</sub>; methyl orange; photocatalysis

**Guochang Chen** is an associate professor of College of Chemistry and Chemical Engineering, Anhui University of Technology, China. His current research interests include photocatalysis and two-dimensional materials.



**Session B4**

**B16**

**16:50 - 17:15 PM Room B June 20**

## Laser direct writing of high-performance micro-supercapacitors on graphene oxide and polymer films

JINGUANG CAI

Institute of Materials, China Academy of Engineering Physics

Jiangyou 621908, Sichuan, PR China

Email: caijinguang@foxmail.com

AKIRA WATANABE

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

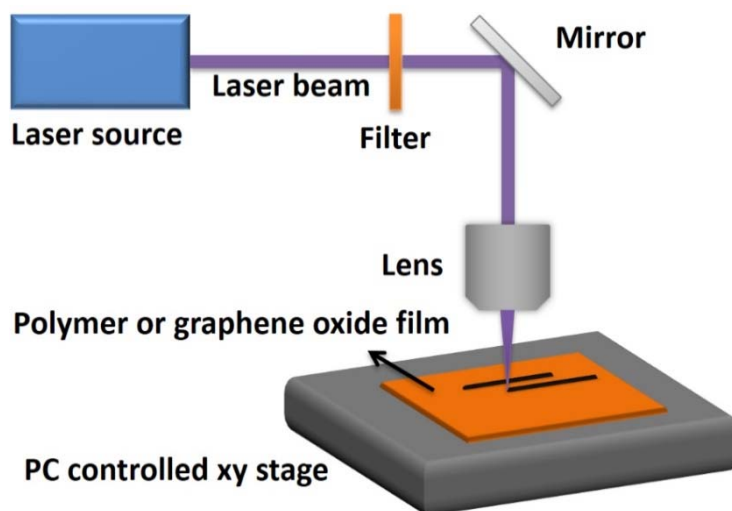
2-1-1, Katahira, Sendai, Japan, 980-8577

Email: watanabe@tagen.tohoku.ac.jp

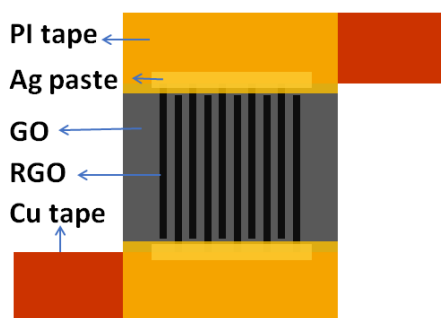
### Abstract

The rapid development of portable miniaturized electronics has improved the research demand for compact energy storage components with high energy and power densities. In recent several years, a new type on-chip energy storage unit, which is called micro-supercapacitor (MSC) with two interdigitated electrodes in the same plane, has attracted much research attention, because MSCs possess not only the advantages of the supercapacitors, such as high power densities, robust cycle performance, pollution-free operation, and maintenance-free features, but also the small size, light weight, and flexibility, as well as the simplified packaging processes and compatibility to the integrated circuits. However, the materials and fabrication methods should be cost-effective, scalable, and compatible with current electronic industries. Carbon materials, especially graphene, which possess high specific surface areas, electrochemical stability, high conductivity, and high mechanical tolerance, can meet the requirement for energy storage unit in flexible wearable devices. Laser induced carbonization from polymers and laser induced reduction of graphene oxide have been reported for the preparation of MSCs due to the high power at the focused area. Compared to the commonly used printing and lithographic techniques, laser direct writing is a non-contact fast single-step fabrication technique with no need for masks, post-processing, and complex clean environments. Moreover, the laser direct writing method has the potential to be integrated to current product lines for commercial use. Therefore, it is necessary and important to study the preparation of high-performance micro-supercapacitors on graphene oxide or polymer films by laser direct writing technique.

In this paper, we will introduce our recent studies on the laser direct writing of high-performance micro-supercapacitors on polyimide and graphene oxide films, which consists of the following several parts: the preparation of carbon MSCs by laser direct writing on polyimide films in air using a continuous-wave blue-violet semiconductor laser (Fig. 1);[1] the improvement of the carbon MSCs by laser direct writing in Ar;[2] the carbon/Au MSC with high-rate charge-discharge capacitive performance;[3] and electrolyte-free high-performance reduced graphene oxide (RGO)-GO-RGO MSCs prepared by laser direct writing on graphene oxide films (Fig. 2).[4]



*Fig. 1 Schematic illustration of the laser direct writing system.*

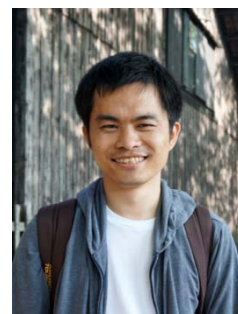


*Fig. 2 Schematic illustrating of a MSC device obtained by laser direct writing. Ag paste was used to make good connection between Cu tape electrodes and RGO lines.*

## References

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**Jinguang Cai** received his Ph.D. degree in physical chemistry from Peking University in 2013. He joined China Academy of Engineering Physics in 2013 and became an associate professor since 2015. He worked as an assistant professor at Institute of Multidisciplinary Research for Advanced Materials, Tohoku University from September 2014 to September 2016. His current research interests include the development of nanostructured materials and fabrication methods for the applications in energy conversion and storage including wearable storage units, self-powered devices, and electrochemical water-splitting.



For more information, please visit <https://scholar.google.com/citations?user=yTLig44AAAAJ>

**Session B4**

**B17**

**17:15 - 17:40 PM Room B June 20**

## How to improve the hydrogen storage of graphene based systems?

SANTHANAMOORTHY NACHIMUTHU, JYH-CHIANG JIANG\*

Department of Chemical Engineering, National Taiwan University of Science and Technology

Taipei 106, Taiwan, ROC

Email: jcjiang@mail.ntust.edu.tw

### Abstract

In the last two decades, the significant efforts have been made to develop alternative energy sources instead of fossil fuels because of increasing CO<sub>2</sub> emissions and the environmental impacts. Besides; hydrogen has been concerned to be an ideal clean energy carrier among the other renewable energy sources because of its environmental friendliness. However, some challenges have to be addressed before hydrogen will become a conventional and commonly available energy carrier. Carbon-based materials such as graphene and carbon nanotubes have been designed for hydrogen storage due to their large surface area, light weight, and tunable properties. Recently, we proposed a new strategy in which we considered three pure transition metal (TM) atoms or/and a combination of two TM atoms and one alkali earth metal atom (AEM) with high, medium and low hydrogen adsorption energies. These different metal atoms are used to decorate the Boron doped graphene sheet (BDG) and investigated their performance towards hydrogen storage capacity through spillover mechanism using first-principles calculations. Our results indicate that that the activation energies for H atom diffusion are much smaller, indicating that a fast H diffusion on this proposed surface can be achieved. These TM and AEM atoms decorated BDG surface can have the maximum hydrogen gravimetric capacity of 6.4% for double-sided adsorptions. To achieve higher gravimetric density, we also considered the Boron and Nitrogen co-doped graphene surface (BNDG) because B–N pair is isoelectronic to the C–C pair. However, controlling the binding strength of considered metal atoms with that of the BNDG surface is an important issue in the application of hydrogen storage. The recent studies have shown that the binding strength between the metal atom and the substrate can be controlled by means of applying an external electric field. Thus, the effects of the external electric field, as well as the effects of applying point charges on the designed medium towards its hydrogen storage capacity, will be discussed.

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**Jyh-Chiang Jiang** graduated from National Taiwan University in 1986 with a B.S. in Chemistry and received his PhD in Chemistry in 1994 from the National Taiwan University. Jiang joined the faculty of National Taiwan University of Science and Technology (NTUST) in 2001. In 2010 he was full Professor in Chemical Engineering Department. Dr. Jiang is Executive Supervisor of the Taiwan Theoretical and Computational Science Association from Sept. 2014. He was the coordinator of NSC- computational chemistry group during Nov. 2009 ~Feb. 2013.



He focuses on the theoretical and computational chemistry study of the heterogeneous catalysis, optoelectronic materials and Li ion batteries. He has worked extensively in the development of combined electronic structure and kinetics methods for simulating processes that involve the reaction mechanisms of H<sub>2</sub> production, Hydrogen storage, NH<sub>3</sub> oxidation on metal oxide surfaces. Dr. Jiang has also involved in High throughput screening of many new materials for Li ion batteries based on quantum mechanics calculation. In addition, he has been active for many years in design of the optoelectronic materials for DSSCs using quantum mechanics simulation.

Session A5

A20

8:00 - 8:25 AM Room A June 21

## Spin texture of flatten Dirac-cone surface state on W(110)

KOJI MIYAMOTO, TAICHI OKUDA

Hiroshima Synchrotron Radiation Center, Hiroshima University

Kagamiyama 2-313, 7390046 Higashi-Hiroshima, Japan

Email: kmiyamoto@hiroshima-u.ac.jp

HENRY WORTELEN, MARKUS DONATH

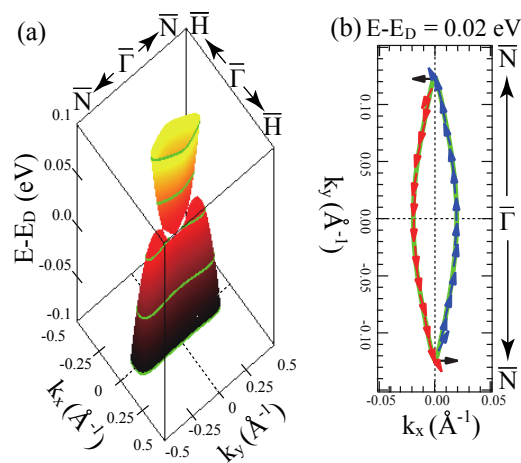
Physikalisches Institut, Westfälische Wilhelms-Universität Münster

Wilhelm-Klemm-Strasse 10, 28149 Münster, Germany

**Abstract**

Topological insulators and Rashba systems with spin-split energy band structure induced by strong spin-orbit interaction have attracted a great attention for the dissipationless spin current transport. The spin orientation of such spin-split state is locked with their crystal momentum and is strongly influenced by the symmetry of surface crystal. However, so-far, most of topological material and Rashba systems are sp-electrons system with  $C_{3v}$  point group symmetry [1].

Recently, we have reported spin polarized Dirac-cone surface state on W(110) with  $C_{2v}$  symmetry [2]. This surface state is formed by d-electrons and strongly influence by two-fold symmetry: the massless and massive band dispersion along  $\overline{\Gamma\text{H}}$  and  $\overline{\Gamma\text{N}}$ . Moreover, by model Hamiltonian based on  $\mathbf{k}\cdot\mathbf{p}$  theorem, it have been predicted that the spin-polarized flatten Dirac-cone surface state shows quasi-one dimensional spin texture as shown in Fig.1 [3]. However, there is no evidence for the spin texture on W(110).



**Fig.1** (a) Energy Contours of the surface state as function of  $k_x$ ,  $k_y$  for energies around crossing point based on model calculation. (c) Spin texture for the constant-energy surface (solid line) at 0.02 eV above crossing point.

The in-plane spin components are shown as arrows.



In this presentation, we have clarified the spin texture of flattened Dirac-cone surface state on W(110) studied by spin- and angle-resolved photoemission spectroscopy. The observed spin texture is in good agreement with our predicted one. This research is the model case of d-electron –based surface state with  $C_{2v}$  symmetry. The finding opens a new avenue in the study of d-electrons-based spin texture with  $C_{2v}$  symmetry. If I have remaining time enough to talk another symmetry surface of tungsten, I will introduce you.

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- [3] K. Miyamoto et al., Massless or heavy due to two-fold symmetry: Surface-state electrons at W(110). *Phys. Rev. B* 86, 161411(R) (2012). doi: 10.1103/PhysRevB.86.161411

**Koji Miyamoto** is assistant professor of Hiroshima Synchrotron Radiation Center at Hiroshima University. He is a Member of Japanese Physics of Society. He received “Young Scientist Award of the Physical Society of Japan” and “Young Scientist Award of the Physical Society of Japan” in the field of spin polarized surface state for topological materials.



His current research interests include topological insulator, weyl semimetal, and superconductivity caused by spin-split band etc... .

For more information, please visit:

<http://seeds.office.hiroshima-u.ac.jp/profile/en.472318719a0d9e04520e17560c007669.html>

**Session A5**

**A21**

**8:25 - 8:45 AM Room A June 21**

## Chiral modes of topological semimetals under magnetic field

XIAO-XIAO ZHANG

Department of Applied Physics, The University of Tokyo,

7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Email: zhang@appi.t.u-tokyo.ac.jp

### Abstract

Topological Dirac/Weyl semimetals, two new quantum phases of matter, attract broad interests from both condensed matter and particle physicists[1,2]. A Dirac (Weyl) semimetal with degenerate (nondegenerate) linear touchings, dubbed as Dirac (Weyl) points, in the electronic band structure is protected by various crystal symmetries (topology)[3-10]. While a Weyl point bears a topological charge in terms of the momentum-space Berry gauge flux, a Dirac point is neutral since it consists of two Weyl points of the opposite topological charge[11]. In addition, the Dirac (Weyl) semimetal exhibits cusps (Fermi arcs) instead of the conventional Fermi ring at the boundary of the Brillouin zone. On the other hand, because of the Landau level formation under an external magnetic field, these band touchings gain to hold massless chiral one-dimensional channels rarely seen outside the discussion of fundamental particles. As a result of the famous chiral anomaly[12-15], the chiral magnetic effect[16] is realized in such systems and is observed as the negative magnetoresistance[17,18].

Here, we try to provide a natural but yet missing analysis of the chiral matter, Weyl semimetal, in terms of the powerful framework of Tomonaga-Luttinger liquid, which enables us to examine the correlation and localization effects largely enhanced in this system under a strong magnetic field. We found new features unique to the 1D channels such as the independent critical exponents for the Greens function and the resistivity, which can be directly compared with experiments of realistic materials. The ubiquitous presence of a large number of Weyl points is also taken into account.

Besides, we consider the Dirac semimetal in the form of a nanowire, i.e., new ingredient of confinement geometry is added to this conventional gapless topological semimetal. Once a magnetic field along the nanowire direction is further applied, there will occur a competition between the effects of the confinement and the magnetic field, which strongly affects how the band gap is opened in the system. Expectedly, the system at finite temperature will show distinct transport features as one turns on and gradually increases the external magnetic field.

There has been an increase of interest recently by the micro- or nano-technology community in considering topological materials emerged in the last decade, whose novel topological properties may bring about new possibilities in various applications. Based on these findings, we hope to clarify a few aspects from the viewpoint of either fundamental science or nano-micro engineering.

### Acknowledgments

This work was supported by JSPS Grant-in-Aids for Scientific Research (No. 16J07545) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.

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**Session A5**

**A22**

**8:45 - 9:10 AM Room A June 21**

## Spin Texture And Spin Injection In A 3D Topological Insulator

W.M. CHEN,\* Y.Q. HUANG, I.A. BUYANOVA

Department of Physics, Chemistry and Biology, Linköping University

S-581 83 Linköping, Sweden

\*Email: wmc@ifm.liu.se

Y.X. SONG, S.M. WANG

State Key Laboratory of Functional Materials for Informatics, CAS Center of Excellence for Superconducting Electronics,

Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences

865 Changning Road, Shanghai 200050, China

### Abstract

One of the most critical steps towards spin functionalized electronics and optoelectronics is to generate and manipulate spin current in a desirable way. In 3D topological insulators (TIs), a strong spin-orbit interaction and the time-reversal symmetry result in spin-momentum locking of the surface electrons, which leads to a unique surface spin texture and the prospect of generating directional and dissipationless spin current running across the surface that is promising for spintronic applications. However, the metallic nature that is often found to be inherent to many 3D TIs due to residual defects has unfortunately imposed a severe obstacle to controlling surface spin current. As a result, very little experimental work has been done so far on this issue. Moreover, since most of the early studies have been limited to Bi<sub>2</sub>Se<sub>3</sub> - a prototypical TI with a rather weak hexagonal warping effect, the contribution of the out-of-plane spin texture to the photocurrent remains elusive so far. In this work, we show that, with circular polarized light, helicity driven photocurrent is obtained in another 3D TI Bi<sub>2</sub>Te<sub>3</sub> that exhibits a stronger hexagonal warping effect. We find the helicity-dependent photocurrent to be sensitive to the incident angle of the light, which could be explained within the framework of the circular photo-galvanic effect (CPGE) by taking into account the spin texture of the topological surface state. By correlating the light incident angle and probing surface current directions, we are able to identify photocurrent components associated with the in-plane and out-of-plane spin texture of the TI and thereby directly uncover the impact of the out-of-plane spin texture on surface spin current promoted by the strong hexagonal warping effect. By exploring the out-of-plane spin texture, we demonstrate spin injection from GaAs to TI and its significant contribution to the surface current [1]. We further show that the spin current of TI can be manipulated by the precession of injected electron spins in an external magnetic field. These discoveries pave the way to not only intriguing new physics but also enriched spin functionalities by integrating TI with conventional semiconductors, such that spin-enabled optoelectronic devices may be fabricated in such hybrid structures.

### References

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**Weimin M. Chen** is Professor of Physics in Linköping University, Sweden, since 1999. He is the founding director of Swedish Interdisciplinary Magnetic Resonance Center and the head of the Functional Electronic Materials group in Linköping University.



His research interests cover a wide range of electronic, optical and spin-related properties of semiconductor materials and nanostructures. His recent research activities focus on spintronic semiconductor nanostructures based on dilute nitrides for room-temperature spintronics, novel III-V quantum dots, quantum-dot molecular structures and nanowires for spintronic and photonic applications, photo-physics of organic solar cells, 3D topological insulators, etc. He is the author of about 660 scientific articles, 74 invited talks at international conferences, 31 review articles and book chapters, and 2 books. He has organized and served as a member of international advisory and program committees of about 30 international conferences. He has also served as a reviewer and a review panelist for 11 Swedish, European and American research councils and funding agencies.

For more information, please visit <http://www.ifm.liu.se/materialphysics/funcel/>.

Session A5

A23

9:10 - 9:35 AM Room A June 21

## Two Dimensional Topological insulators: Progress and Prospects

LIANGZHI KOU

School of Chemistry, Physics and Mechanical Engineering

Queensland University of Technology, Brisbane, Australia

Email: Liangzhi.kou@qut.edu.au

### Abstract

2D topological insulator is a new state of quantum matter with the protected metallic edge state inside a bulk energy gap, which is spin-locked due to the protection of the time-reversal symmetry, leading to dissipationless transport edge channels. It is thus highly promising and useful for spintronics application and nanodevices design, and therefore attracting extensive research for the fundamental investigations. Here we first introduce two general approaches to achieve large gap topological insulators, namely SOC enhancement via building quantum wells and intrinsic strong SOC to induce topological phase transition. A large family of 2D TIs based on the two methods is therefore predicted. We then summarize the current progress of 2D TI research, and assess the current status and challenges of experimental synthesis and potential device applications of 2D TIs and discuss prospects of exciting new opportunities for future research and development of this fascinating class of materials.

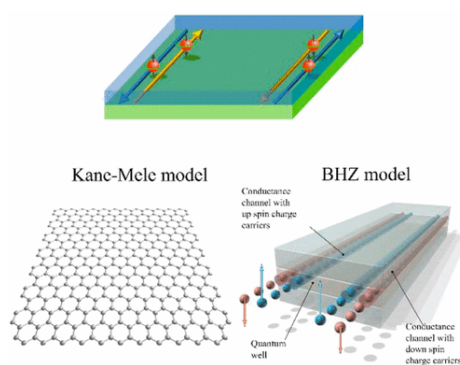


Fig.1

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**Liangzhi Kou** is a lecturer and ARC DECRA fellow in Queensland University of Technology. He got his PhD degree in 2011. From 2012 to 2014, he was an Alexander von Humboldt research fellow and worked with Professor Thomas Frauenheim at University of Bremen in Bremen Center of Computational Materials Science (BCCMS). From 2014 to 2015, he was a Postdoctoral Fellow working with Prof. Sean Smith of University of New South Wales, Australia. His research interests are topological insulator and two-dimensional materials.



For more information, please visit: <http://staff.qut.edu.au/staff/koul/>.



**Session A5**

**A24**

**9:35 - 10:00 AM Room A June 21**

## Charge-current induced spin polarization in BiSbTeSe<sub>2</sub> topological insulators

FAN YANG, SUBHAMOY GHATAK, A. A. TASKIN, YOICHI ANDO

Institute of Physics II, University of Cologne  
Zuelpicher Strasse 77, 50937 Koeln, Germany  
Email: yang@ph2.uni-koeln.de

YUICHIRO ANDO, MASASHI SHIRAISHI

Department of Electronic Science and Engineering, Kyoto University  
Katsura, Nishikyo-ku., Kyoto 615-8510, Japan

KOUJI SEGAWA, YASUSHI KANAI, KAZUHIKO MATSUMOTO

Institute of Scientific and Industrial Research, Osaka University  
8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan

ACHIM ROSCH

Institute of Theoretical Physics, University of Cologne  
Zuelpicher Strasse 77, 50937 Koeln, Germany

### **Abstract**

The surface states of 3D topological insulators (TIs) possess a helical spin texture in which the spin and momentum are perpendicularly locked to each other. Due to this spin-momentum locking, a net spin polarization can be induced by a charge current and vice versa. However, topological surface states are expected to give rise to only one type of spin polarization for a given current direction, which has been a limiting factor for spin manipulations. In this talk we report that in devices based on the bulk-insulating topological insulator BiSbTeSe<sub>2</sub>, two different kinds of spin polarizations were observed in different devices: The spin polarization expected from the topological surface states was detected in a heavily electron-doped device, whereas the opposite polarization was reproducibly observed in devices with low carrier densities. [1] We propose that the latter type of spin polarization stems from topologically-trivial two-dimensional states with a large Rashba spin splitting, which are caused by a strong band bending at the surface of BiSbTeSe<sub>2</sub> beneath the ferromagnetic electrode used as a spin detector. This finding paves the way for realizing the "spin transistor" operation in future topological spintronic devices.

**References**

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**Fan Yang** is a postdoctoral researcher in physics at Institute of Physics II, University of Cologne, Germany.

His current research mainly focuses on micro-devices based on topological materials, such as topological spintronic devices, Josephson junctions and gated topological-insulator films.

For more information, please visit:

<http://www.ph2.uni-koeln.de/ando-members.html>



**Session A6**

**A25**

**10:20 - 10:45 AM Room A June 21**

## Novel Topological Phase with a Zero Berry Curvature

FENG LIU AND KATSUNORI WAKABAYASHI

Department of Nanotechnology for Sustainable Energy  
School of Science and Technology, Kwansai Gakuin University  
Email: ruserzzz@gmail.com

### **Abstract**

Recalling the scenario of Aharonov-Bohm effect that electrons experience a phase shift induced by a magnetic vector potential in spite of a zero-magnetic field, we have a similar story in topological version to tell here, where the magnetic field and the magnetic vector potential are replaced by their geometric counterparts, Berry curvature and Berry connection, respectively.

Starting from a simple two-dimensional tight-binding model with two types of hopping, i.e. intercellular  $\gamma$  and intracellular hopping  $\gamma'$  based on square lattice, we show that nontrivial topological phase emerges when  $|\gamma| < |\gamma'|$  under a zero Berry curvature. Our work offers a new way to design topological materials without Berry curvatures [1].

### **References**

[1] F. Liu and K. Wakabayashi. Phys. Rev. Lett. 118, 076803 (2017).

**Feng Liu** is a postdoctoral researcher of Kwansei Gakuin University.

His current research interests include topological insulators, graphene-related materials, and valleytronics.

For more information, please visit  
[https://www.researchgate.net/profile/Feng\\_Liu115](https://www.researchgate.net/profile/Feng_Liu115).



**Session A6**

**A26**

**10:45 - 11:10 AM Room A June 21**

**2D materials-assisted fiber device as a novel nonlinear optical platform for multiwavelength ultrafast photonics**

BO GUO

Key Lab of In-Fiber Integrated Optics of Ministry of Education, Harbin Engineering University

Harbin Engineering University, No.145 Nantong Street, Nangang District, Harbin, China

Email: guobo512@163.com

**Abstract**

Since the first report of graphene mode-locked laser in 2009, the research on mode-locked lasers with 2D materials, such as graphene, topological insulators (TIs), transition metal dichalcogenides (TMDs) and black phosphorus (BP) as saturable absorber is booming. Here, we summary the recent progress on the exploitation of these materials in multiwavelength ultrafast lasers and verified that 2D materials-assisted fiber device is an ideal platform for nonlinear pulse dynamics study. Versatile pulse pattern is also reviewed. Finally, we present an outlook of multiwavelength lasers regarding current challenges and future application opportunities.

**Bo Guo** is currently a Lecturer of Key Lab of In-Fiber Integrated Optics of Ministry of Education, School of Science, Harbin Engineering University. He received the B.S. degree in physics from Henan University, Kaifeng, China, in 2005. He then moved to the Harbin Institute of Technology and received the M.S. and Ph.D. degrees in optics and physical electronics in 2011 and 2015, respectively.



His current research interests include 2D Materials optoelectronic device, mode-locked/Q-switched laser technology, mid-infrared laser technology and nonlinear physics. He published nearly 20 papers on various international journals.

For more information, please visit <http://www.escience.cn/people/guobo/index.html>.

**Session A6**

**A27**

**11:10 - 11:35 AM Room A June 21**

## Quantum phase transitions and order parameters of a topological insulator

Yan-Chao Li<sup>1,2</sup>

<sup>1</sup> University of Chinese Academy of Sciences, Beijing, China

<sup>2</sup> Beijing Computational Science Research Center, Beijing, China

Email: [ycli@ucas.ac.cn](mailto:ycli@ucas.ac.cn)

### **Abstract**

Using quantum entanglement, quantum coherence, and the reduced density matrix, we study the quantum phase transitions and propose order parameters for the phases of a topological insulator, specifically a spinless Su-Schrieffer-Heeger (SSH) model, and consider the effect of short-range interactions. All the derived order parameters and their possible corresponding quantum phases are verified by the entanglement entropy and electronic configuration analysis results. The order parameter appropriate to the topological regions is further proved by calculating the Berry phase under twisted boundary conditions. It is found that the topological nontrivial phase is robust to the introduction of repulsive intersite interactions and can appear in the topological trivial parameter region when appropriate interactions are added.



**Yan-Chao Li**, University of Chinese Academy of Sciences. Associate Professor.

He received his Ph.D. from Institute of Semiconductors, Chinese Academy of Sciences (2010), then went to Beijing Computational Science Research Center as a postdoc (2010-2012). In 2013 he joined College of Materials Science and Opto-Electronic Technology in University of Chinese Academy of Sciences.



His main research interests focus on quantum phase transitions of one-dimensional systems, strongly correlated systems, and disorder and magnetic field effects in superconductors. He pointed out a density-matrix Loschmidt echo method, and proved it is a convenient way to connect with the density matrix renormalization group technique (DMRG) to detect different types of quantum phase transition. In addition, he analyzed the capability of the pairwise quantum discord (QD) in detecting quantum phase transitions (QPTs) at both zero and finite temperatures, and found that, in contrast to entanglement, it can be used to detect critical points of QPTs at a relative high temperature. Up to now, as a first order author, he has published more than 15 papers, including *Phy. Rev. A*, *Phy. Rev. B*, *Sci. Rep.*, and so on.

For more information, please visit <http://js.caseducation.cn/10/homepage>

## Session A6

A28

11:35 - 12:00 PM Room A June 21

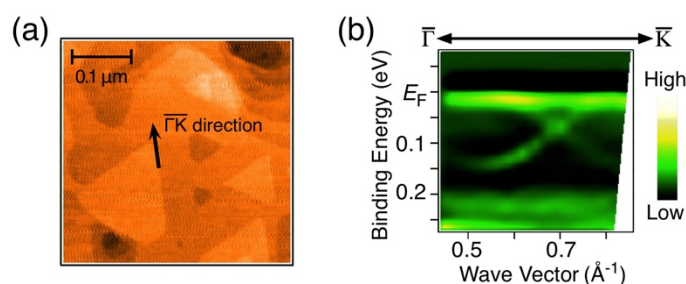
## One-dimensional edge states with spin splitting in bismuth

A. TAKAYAMA<sup>1\*</sup>, T. SATO<sup>2</sup>, S. SOUMA<sup>3</sup>, T. OGUCHI<sup>4</sup>, AND T. TAKAHASHI<sup>2,3</sup><sup>1</sup>Department of Physics, The University of Tokyo, Bunkyo-ku 113-0033, Japan<sup>2</sup>Department of Physics, Tohoku University, Sendai 980-8578, Japan<sup>3</sup>WPI Research Center, Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan<sup>4</sup>Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan

\*Email: a.takayama@surface.phys.s.u-tokyo.ac.jp

**Abstract**

A two-dimensional (2D) system with strong spin-orbit coupling like a topological-insulator surface and semiconductor-heterostructure interface has provided a useful platform for realizing novel quantum phenomena applicable to advanced spintronic devices. 1 bilayer (BL) bismuth is theoretically predicted to be 2D topological insulator and have a spin-polarized state at edge [1,2]. However, it is not certain experimentally because to prepare a free-standing 1 BL bismuth is very difficult. Here we challenged to observe a spin-polarized electric state at edge by different approach. As observed by the atomic force microscopy (AFM) of our Bi thin film [Fig. 1(a)], triangular-shaped bismuth BL islands with typically  $\sim 0.1 \mu\text{m}$  edge length are formed on the top surface of the Bi thin film, and the edge of each island runs along the  $\Gamma\text{K}$  direction in the  $k$  space. And we have also observed the 1D band dispersion from the edge state of bismuth islands measured by ARPES. In this presentation, we show the result of ARPES and spin-resolved ARPES for bismuth thin film, and discuss the origin of the 1D spin-splitting band compared with our first-principles band-calculations.



**Fig.1** (a) AFM image measured at 300 K in Air and (b) Band dispersion near  $E_F$  along  $\Gamma\text{K}$  line measured at 30 K in UHV for a Bi thin film, respectively.

**References**

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**Akari Takayama** is Assistant Professor of Department of Physics in The University of Tokyo. Member of JPS, SSSJ, and JSSRR. This work was supported by the JSPS KAKENHI Grant Number JP15K17464, and Inoue research award.



Current research: topological insulator, Rashba effect, superconductivity of surface-superstructure

<http://www-surface.phys.s.u-tokyo.ac.jp/entrance.html>

Session A6

A29

12:00 - 12:25 PM Room A June 21

## Magnetic Topological Insulators and Their Heterostructures

XUFENG KOU<sup>1,2</sup>, LEI PAN<sup>2</sup>, QINGLIN HE<sup>2</sup>, YABIN FAN<sup>2</sup>, AND KANG L. WANG<sup>2,3,4</sup>

<sup>1</sup>School of Information Science and Technology, ShanghaiTech University

<sup>2</sup>Department of Electrical Engineering, <sup>3</sup>Department of Physics, and <sup>4</sup>Department of Materials Sciences and Engineering, University of California Los Angeles

Email: kxf2323@gmail.com

### Abstract

When magnetic order is introduced into topological insulators (TIs), the time-reversal-symmetry is broken, and the non-trivial topological surface is driven into a new massive Dirac-fermions state. By adjusting the Fermi level position, quantum anomalous Hall effect (QAHE) emerges in the Cr-doped  $(\text{BiSb})_2\text{Te}_3$  samples where dissipationless chiral edge conduction is realized in the macroscopic millimeter-size devices without the presence of an external magnetic field, and the stability of the dissipationless chiral edge conductance is well-maintained as the film thickness varies across the 2D hybridization limit. By further manipulating the topological surface gap, we realize the metal-to-insulator quantum phase transition in the system.

In addition to the uniform magnetic TIs, our recent work on several magnetic TI based heterostructures will be presented. First, in the TI/Cr-doped TI system, we demonstrate that the spin-orbit torque is highly efficient that the critical charge current density required for the magnetization switching is three orders of magnitude smaller than that of heavy metals. In addition, by constructing novel AFM/TI heterostructures, we realize emergent interfacial magnetic effects, which can be tailored through artificial structural engineering. Finally, by introducing additional superconductivity (SC), we observe the presence of the chiral Majorana edge mode in the QAHE-SC hybrid system. All these exotic magnetic TI-based phenomena will serve as fundamental steps to further explore the TRS-breaking TI systems.

**Xufeng Kou** received his BS degree (with honor) in Chu Kochen Honors College and Optical Engineering from Zhejiang University (2009). From 2009 to 2014, he received his MS and PhD degrees in Electrical Engineering from University of California, Los Angeles. In February 2016, he joined ShanghaiTech University as a tenure-track assistant professor in the School of Information Science and Technology. So far, Dr. Kou has co-authored 47 peer-reviewed journal papers including *Nature Mater*, *Nature Nano.*, *Nature Comm.*, *Phys. Rev. Lett.*, *Nano Lett.*. He also holds several awards including the Qualcomm Innovation Fellowship (2012), Chinese Outstanding Student Abroad Scholarship (2013), Distinguished PhD Dissertation Award of UCLA (2015), and Chinese 1000 Young Talents Award (2017).



His current research interests include nano-electronics, spintronics and, topological quantum matters

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Session A7

A30

14:00 - 14:25 PM Room A June 21

## Green Semiconductor Vertical-Cavity Surface-Emitting Lasers based on Quantum Dots

BAOPING ZHANG, YANG MEI, RONGBIN XU, ZHIWEI ZHENG, HAO LONG, LEIYING YING

Department of Electronic Engineering, Xiamen University

Xiamen, China

Email: bzhang@xmu.edu.cn

### Abstract

Green VCSELs emitting in the spectral range from 491.8 nm to 565.7 nm, covering most of the 'green gap', are demonstrated. These devices are featured with low threshold current and CW lasing at room temperature. A few technologies such as laser liftoff of sapphire substrate, the removal of high-defect GaN buffer and Cu plating to increase the heat dissipation. Two dielectric DBRs were adopted as the cavity mirrors. The results presented here open up opportunities to design and fabricate semiconductor green lasers with excellent performance that may lead to wide-gamut, low consumption power and compact displays and projectors. The VCSELs could also be bonded on to Si for integration with other optoelectronic devices/circuits.

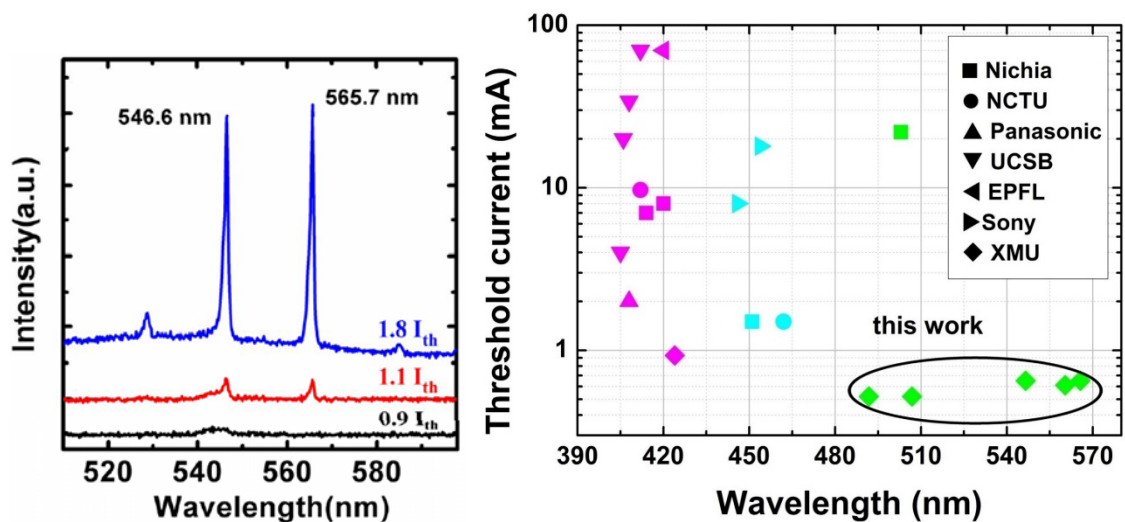


Fig.1 Lasing spectra(left)in this work and comparison(right) of threshold currents with literatures.

**References**

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**BAOPING ZHANG** is Professor of Electronic Engineering and Director of Department of Electronic Engineering, Xiamen University. He received the B.S. degree in physics in 1983 from Lanzhou University, M.E. degree in electronic engineering in 1986 from Hebei Semiconductor Research Institute (HSRI), China, and the Dr. Eng. degree in applied physics in 1994 from the University of Tokyo, Japan. He engaged in research in HSRI , Institute of Physical and Chemical Research (RIKEN), and Sharp Corporation, Japan. In 2006, he joined the Department of Physics, Xiamen University, Xiamen, China, as a distinguished professor. Since 2013, he moved to the Department of Electronic Engineering. His research interests include wide-gap semiconductor materials, light-emitting diodes, vertical-cavity surface-emitting lasers, solar cells, nanostructures.



Session A7

A31

14:25 - 14:50 PM Room A June 21

## Titanium Dioxide Films with Pure Anatase Phase Synthesized by Mist Chemical Vapour Deposition

CHAOYANG LI, QIANG ZHANG, LILIN XIE

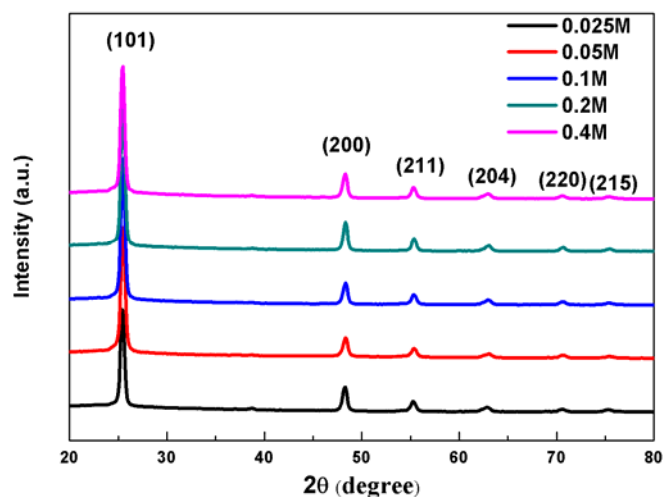
School of System Engineering, Kochi University of Technology

185 Miyanokuchi Tosayamada cho Kami City, Kochi 782–8502, Japan

Email: li.chaoyang@kochi-tech.ac.jp

### Abstract

Pure anatase structured TiO<sub>2</sub> films were successfully synthesized by a novel fine channel mist chemical vapour deposition which is a vacuum free, low temperature method [1]. The effects of TTIP concentration on the morphological, structural and optical properties of TiO<sub>2</sub> films were investigated. It was confirmed that anatase crystallinity of TiO<sub>2</sub> film increased with the increase of TTIP concentration. Fig. 1 showed that XRD patterns of TiO<sub>2</sub> thin films which were synthesized with the different concentration of TTIP in ethanol varying from 0.025 to 0.4 mol/L. The high catalytic activity will be expected by using obtained stable anatase TiO<sub>2</sub> films.



**Fig.1** XRD patterns of TiO<sub>2</sub> films synthesized at TTIP concentration of 0.025, 0.05, 0.1, 0.2, and 0.4 mol/L.

### References

[1] T. Kawaharamura, and S. Fujita, “An approach for single crystalline zinc oxide thin films with fine channel mist chemical vapor deposition method” *Phys. Status Solidi C*, 5 (2008) 31383140.

**Chaoyang Li** is currently a professor at Kochi University of Technology, Japan. She received the B.S degree in physics, the M.S degree in microelectronics and solid state electronics from Heilongjiang University, China. She received the Ph.D degree in Electrical Engineering at the Kochi University of Technology, Japan. She has worked on the semiconductor growth, physics, processing and devices for many years. She also contributed to the hundreds of scientific international journals and international conferences. She has led and participated in many research projects. Her current research interests include nanotechnology, sensor and photovoltaic devices.



**Session A7**

**A32**

**14:50 - 15:15 PM Room A June 21**

## Tuning solar absorptance and reflection of high-temperature solar spectrally selective surfaces

FENG CAO

School of Science, Harbin Institute of Technology Shenzhen Graduate School  
Shenzhen, 518055, China,  
Email: caofeng@hit.edu.cn

QIAN ZHANG

School of Materials Science and Engineering, Harbin Institute of Technology Shenzhen Graduate School, Shenzhen, 518055, China  
Email: zhangqf@hit.edu.cn

ZHIFENG REN

Department of Physics and TeSUH, University of Houston, Houston, TX 77204, USA  
Email: zren@uh.edu

### Abstract

Spectrally-selective solar absorbers are widely used in solar hot water and concentrating solar power (CSP) systems.<sup>[1,2]</sup> However, the performance at high temperatures (>450 °C) is still not satisfactory due to their high infrared (IR) emittance and long term thermal stability. Recent progress on cermet-based solar absorbers has shown promising temperature thermal stability and wavelength selectivity. Thus, here we explore W-Ni-Al<sub>2</sub>O<sub>3</sub>, W-Ni-YSZ (yttria-stabilized-zirconia) and W-Ni-SiO<sub>2</sub> cermet based spectrally selective surfaces for high-temperature solar absorber applications.<sup>[3,4]</sup> The developed multilayer selective surfaces are deposited on a polished stainless steel substrate comprising two sunlight absorbing cermet layers with different W-Ni volume fraction inside the dielectric matrix, one or two anti-reflection coatings (ARCs) and one tungsten IR reflection layer for reduced IR emittance and improved thermal stability.

Regarding the W-Ni-Al<sub>2</sub>O<sub>3</sub> cermet based solar absorbers; we observed a detrimental change in the morphology, phase, and optical properties if the cermet layers are deposited on a stainless steel substrate with a thin nickel adhesion layer, which is due to the diffusion of iron atoms from the stainless steel into the cermet layer forming a FeWO<sub>4</sub> phase. A 100 nm thick tungsten layer can suppress the degradation of the optical properties at high temperatures and lowers the emittance relative to the stainless steel substrate, which improves the spectral selectivity of the solar absorber. We experimentally demonstrated a solar absorber with a solar absorptance of ~0.9 and total hemispherical emittance of ~0.15 at an operating temperature of 500 °C.

The fabricated W-Ni-YSZ cermet based solar absorbers are tested for their long term thermal stability at 600 °C. A distinct change in surface morphology of the solar absorbers with high oxygen deficiency in their YSZ-ARC layers, suggests to causing the degradation of the optical properties at high

temperature. The oxygen deficiency can be effectively overcome through increasing the oxygen partial pressure during sputtering, which leads to a stable solar absorber with an experimentally demonstrated solar absorptance of  $\sim 0.91$  and a total hemispherical emittance of  $\sim 0.13$  at  $500\text{ }^{\circ}\text{C}$ .

We also developed a new kind of absorber that reflects a certain range of wavelength and absorbs the rest of the whole solar spectra.<sup>[5]</sup> The absorbed part is used for electrical power generation by steam engine and the reflected part is used for solar photovoltaic conversion. The thermal energy can be easily stored for later conversion to provide electrical power around the clock without worrying the Sun's night time.

### **References:**

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**Feng Cao** is an Associate Professor of Physics of Harbin Institute of Technology Shenzhen Graduate School. He received his Ph. D. degree in Physics from the Hong Kong Polytechnic University in 2012. He worked as a Postdoctoral fellow at the Boston College for one year (2012) and then moved to the University of Houston as a research associate (2013-2016).



His current research interests include Optical Functional Films, Solar Energy Photothermal Conversion, and Infrared Radiation Controlling.

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[http://www.hitsz.edu.cn/index.php?s=/index/news\\_view/fid/263/eid/1758.html](http://www.hitsz.edu.cn/index.php?s=/index/news_view/fid/263/eid/1758.html).

**Session A7**

**A33**

**15:15 - 15:40 PM Room A June 21**

## **Broadband Optical Absorption Based on Plasmonic Nanostructures**

QIANG LI AND MIN QIU

State Key Laboratory of Modern Optical Instrumentation, College of Optical Science and Engineering, Zhejiang University,  
Hangzhou 310027, China  
Email: qiangli@zju.edu.cn

### **Abstract**

Plasmonic metamaterial absorbers have garnered significant interest due to their unique ability to trap light beyond diffraction limit and potential applications in energy harvesting and information processing. Especially, the broadband absorbers show fascinating applications in photovoltaics and thermophotovoltaics, bolometers, thermal emitters, and photodetectors. In this talk, I will review our recent work on broadband optical absorption based on plasmonic based on ultra-thin metal-insulator-metal (MIM) plasmonic absorbers [1-2].

### **References**

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- [2] X. X. Chen, H. M. Gong, S. W. Dai, D. Zhao, Y. Q. Yang, Q. Li, and M. Qiu Near-infrared broadband absorber with film-coupled multilayer nanorods. *Optics Letters*, 38: 2247-2249 (2013).

**Dr. Qiang Li** received the B.Sc. degree and M. Eng from the Harbin Institute of Technology, Harbin, China, in 2005 and 2007, respectively. He obtained the Ph.D. degree in Microelectronics and Applied Physics from the Royal Institute of Technology (KTH), Stockholm, Sweden, in 2011. In 2011 he joined College of Optical Science and Engineering, Zhejiang University, as an assistant professor. He became an associate professor in 2013. His research interest focuses on integrated photonics and nanophotonics. He has published over 60 reviewed research papers, with a total citation of over 700. His h-index is 17.



For more information, please visit [ipnp.zju.edu.cn](http://ipnp.zju.edu.cn).



**Session A8**

**A34**

**16:00 - 16:25 PM Room A June 21**

## **Unsteady flow and heat transfer of MHD nano-liquid thin film over a stretching sheet under thermocapillarity effect**

YAN ZHANG, MIN ZHANG, YU BAI

School of Science, Beijing Key Laboratory of Functional Materials for Building Structure and Environment Remediation, Beijing University of Civil Engineering and Architecture

No.1, Zhanlanguan Road, Xicheng District, Beijing, China

Email: zhangyan1@bucea.edu.cn

### **Abstract**

The unsteady boundary layer flow and heat transfer of Cu-water nanofluid thin film over a stretching sheet have been investigated. The thermocapillarity effect is taken into consideration. The surface tension is assumed to vary linearly with temperature. The governing partial differential equations are transformed into the nonlinear ordinary differential equations by similarity transformation. The numerical and analytical solutions are obtained simultaneously using the shooting technique and homotopy analysis method (HAM). The influences of various relevant parameters on the flow field are elucidated through graphs and tables. The results illustrate that the copper volume fraction and Marangoni surface tension have more remarkable effects.

### **References**

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**Yan Zhang** is Professor of Mathematics and Deputy Laboratory Director of Beijing Key Laboratory of Functional Materials for Building Structure and Environment Remediation.

Her current research interests include Nano fluid, Heat and Mass Transfer.

For more information, please visit  
<http://sci.bucea.edu.cn/yjsjy/yjsds/28289.htm>



*Session A8*

*A35*

*16:25 - 16:50 PM Room A June 21*

## Focusing and Separating Diamagnetic Microparticles with Multiphase Ferrofluids

CHENG WANG\*, RAN ZHOU

Department of Mechanical and Aerospace Engineering,

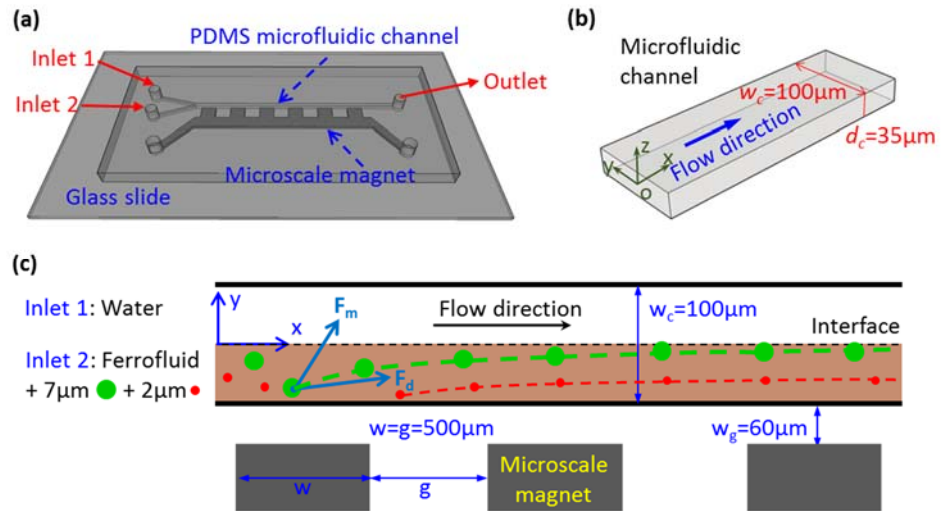
Missouri University of Science and Technology

400 W. 13th St., MO 65409, USA

Email: wancheng@mst.edu

### **Abstract**

Ferrofluids have demonstrated great potential for a variety of manipulations of diamagnetic (or non-magnetic) micro-particles/cells in microfluidics, including sorting, focusing, and enriching. By utilizing size-dependent magnetophoresis velocity, most of the existing techniques employ single phase ferrofluids to push particles towards channel walls. In this work, we demonstrate a novel strategy for focusing and separating diamagnetic micro-particles by using the laminar fluid interface of two co-flowing fluids -- a ferrofluid and a non-magnetic fluid [1]. As shown in Fig. 1, next to the microfluidic channel, microscale magnets are fabricated to generate strong localized magnetic field gradients and forces. Due to the negative magnetophoresis force, diamagnetic particles suspended in the ferrofluid phase migrate across the ferrofluid stream at size-dependent velocities. Because of the low Reynolds number and high Peclet number associated with the flow, the fluid interface is sharp and stable. When the micro-particles migrate to the interface, they are accumulated near the interface, resulting in effective focusing and separation of particles. We investigated several factors that affect the focusing and separation efficiency, including susceptibility of the ferrofluid, distance between the microfluidic channel and microscale magnet, and width of the microfluidic channel. This concept can be extended to multiple fluid interfaces. As an example, complete separation of micro-particles was demonstrated by using a three-stream multiphase flow configuration.



**Fig.1** Overview of the device and principle of particle separation. (a) a two-inlet microchannel and microscale magnets; (b) dimensions of the main fluidic channel. (c) basic principle of particle movement in a ferrofluid.

## References

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**Cheng Wang** has been an assistant professor of Mechanical Engineering at Missouri University of Science and Technology since 2014. He received his Ph.D. in mechanical engineering from the University of Illinois at Urbana-Champaign (UIUC) in 2013. His research interests include microfluidics, droplet and bubble dynamics, acoustic streaming flows, and microscale magneto-fluidics.

For more information, please visit <http://web.mst.edu/~wancheng/>.



**Session A8**

**A36**

**16:50 - 17:15 PM Room A June 21**

## **Porous WO<sub>3</sub> on FTO Substrates: Fabrication and Photoelectrochemical Water Oxidation Performance**

LIUYUAN HAN, CHANGLONG CHEN,\* RANRAN LU, Qinglong Liu  
School of Chemistry and Chemical Engineering, University of Jinan, 250022  
No. 336, West Road of Nan Xinzhuang, Jinan, Shandong, P. R. China  
Email: chm\_chencl@ujn.edu.cn

### **Abstract**

WO<sub>3</sub>·0.33H<sub>2</sub>O films composed of nanorod-like WO<sub>3</sub>·0.33H<sub>2</sub>O single crystals were firstly deposited hydrothermally on fluorine doped tin oxide substrates and then were annealed at 500°C to convert to WO<sub>3</sub>. Employing a photoelectrochemical etching process the WO<sub>3</sub> nanorods were successfully etched to form porous nanostructures. When used as photoanodes, the porous WO<sub>3</sub> films showed much enhanced photoelectrochemical water splitting performance in comparison with the non-etched WO<sub>3</sub> films: under the illumination of simulated solar light and without using any oxygen evolution co-catalysts, the photocurrent increased from 0.06 mA/cm<sup>2</sup> to 0.23 mA/cm<sup>2</sup> at 1.23 V vs. RHE and the overpotential decreased from 1.0 V to 0.8 V vs. RHE. It suggests that the simple photoelectrochemical etching is an effective way to form porous nanostructures on conductive substrates, which is expected to be expanded to prepare other semiconductor porous structures to increase their specific area thereby enhancing their corresponding functional properties.

**Keywords:** Porous WO<sub>3</sub>; Photoelectrochemical; Water Splitting; Water Oxidation

**Changlong Chen** is Professor of Material Chemistry of University of Jinan.

His current research interests include Water Splitting, Solar Fuel, Photocatalysis.

For more information, please visit:

<http://chem.ujn.edu.cn/showjiaoshi.asp?jiaoshixm=%E9%99%88%E9%95%BF%E9%BE%99>



**Session A8**

**A37**

**17:15 - 17:40 PM Room A June 21**

## **H<sub>2</sub>-evolving SWCNT Photocatalysts for Effective Use of Solar Energy**

KIKI KURNIAWAN, NORITAKE MURAKAMI, YUTO TANGO, TAKUMI IZAWA, KAKERU NISHIKAWA, KEN WATANABE, HIDEAKI MIYAKE, TOMOYUKI TAJIMA, YUTAKA TAKAGUCHI\*

Graduate School of Environmental & Life Science, Okayama University

3-1-1 Tsushima-Naka, Kita-Ku, Okayama, 700-8530, Japan

Email: yutaka@cc.okayama-u.ac.jp

### **Abstract**

Effective hydrogen evolution from water using SWCNT photocatalyst under near-infrared (NIR) light illumination was demonstrated. H<sub>2</sub> evolution reactions of 1.2 and 0.40 μmol/h were observed upon chirality-selective photoexcitation by the use of monochromatic light irradiation at 680 and 1000 nm, which are the E<sub>22</sub> and E<sub>11</sub> absorptions of (8,3)SWCNT, respectively, by the use of SWCNT/fullerodendron photosensitizer in the presence of a sacrifice donor, an electron relay, and a co-catalyst. Apparent quantum yields of this reaction were 0.17 (at 680 nm) and 0.073 (at 1000 nm), respectively. The result provides the first example of photocatalytic H<sub>2</sub> evolution reaction triggered by E<sub>11</sub> photoexcitation of SWCNTs, and clearly shows the usefulness of SWCNTs in the light absorber for NIR light, which is the second main component of solar radiation.



**Yutaka Takaguchi** is Professor of Chemistry at Graduate School of Environmental and Life Science, Okayama University, JAPAN. He is also Visiting Professor at Graduate School of Sciences and Technology for Innovation, Yamaguchi University, JAPAN. His current research interests include (1) SWCNT photocatalysts, (2) SWCNT drug delivery/bio-imaging systems, (3) photoproperties of organic/inorganic nanohybrids, and (4) Stimuli responsive organic semiconductors.



For more information, please visit <http://www.ecm.okayama-u.ac.jp/organic/>.

Session A8

A38

17:40 - 18:05 PM Room A June 21

## One-Dimensional Nanomaterials for Energy Storage

LIQIANG MAI\*, LIN XU

122 Luoshi Road, Wuhan 430070, Hubei, China

\*Email: mlq518@whut.edu.cn

### Abstract

One-dimensional nanomaterials can offer large surface area, facile strain relaxation upon cycling and efficient electron transport pathway to achieve high electrochemical performance. Hence, nanowires have attracted increasing interest in energy related fields. We designed the single nanowire electrochemical device for in situ probing the direct relationship between electrical transport, structure, and electrochemical properties of the single nanowire electrode to understand intrinsic reason of capacity fading. The results show that during the electrochemical reaction, conductivity of the nanowire electrode decreased, which limits the cycle life of the devices.<sup>1</sup> We have fabricated hierarchical MnMoO<sub>4</sub>/CoMoO<sub>4</sub> heterostructured nanowires by combining "oriented attachment" and "self-assembly".<sup>2</sup> The asymmetric supercapacitors based on the hierarchical heterostructured nanowires show a high specific capacitance and good reversibility with a cycling efficiency of 98% after 1,000 cycles. Then, we designed the general synthesis of complex nanotubes by gradient electrospinning, including Li<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub>, Na<sub>0.7</sub>Fe<sub>0.7</sub>Mn<sub>0.3</sub>O<sub>2</sub> and Co<sub>3</sub>O<sub>4</sub> mesoporous nanotubes, which exhibit ultrastable electrochemical performance when used in lithium-ion batteries, sodium-ion batteries and supercapacitors, respectively.<sup>3</sup> In addition, we have successfully fabricated a field-tuned hydrogen evolution reaction (HER) device with an individual MoS<sub>2</sub> nanosheet to explore the impact of field effect on catalysis.<sup>4</sup> We also constructed a new-type carbon coated K<sub>0.7</sub>Fe<sub>0.5</sub>Mn<sub>0.5</sub>O<sub>2</sub> interconnected nanowires through a simply electrospinning method. The interconnected nanowires exhibit a discharge capacity of 101 mAh g<sup>-1</sup> after 60 cycles, when measured as a cathode for K-ion batteries.<sup>5</sup> Our work presented here can inspire new thought in constructing novel one-dimensional structures and accelerate the development of energy storage applications.

### Reference

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**Liqliang Mai** PhD, Chair Professor, Cheung Kong Scholar of Materials Physics and Chemistry, Distinguished Young Scholar of the National Science Fund of China, Executive Dean of International School of Materials Science and Engineering in Wuhan University of Technology.

He is the winner of the National Natural Science Fund for Distinguished Young Scholars, China Youth Science and Technology Award, and Guanghua Engineering Award. He also won Hundred, Thousand, and Ten Thousand Talents Project, Nanoscience Research Leader award, Ten Thousand Talents Project, Person of the Year (2014) of Scientific Chinese, the First Prize for Hubei Natural Science Award, Hubei Youth Five Four Medal, etc.



His current research interests include nano energy materials and micro/nano devices.

For more information, please visit <http://mai.group.whut.edu.cn/>

**Session B5**

**B19**

**8:00 - 8:25 AM Room B June 21**

## Photocatalytic elimination of organic chemicals and aerosol-associated influenza virus infectivity in the air

KIMIYASU SHIRAKI<sup>1</sup>, HIROSHI YAMADA<sup>1</sup>, YOSHIHIRO YOSHIDA<sup>1</sup>, AYUMU OHNO<sup>1</sup>, TERUO WATANABE<sup>2</sup>, TAKAFUMI WATANABE<sup>2</sup>, HIROYUKI WATANABE<sup>2</sup>, HIDEMITSU WATANABE<sup>2</sup>, MASAO YAMAGUCHI<sup>2</sup>, FUMIO TOKUOKA<sup>3</sup>, SHIGEATSU HASHIMOTO<sup>4</sup>, MASAKAZU KAWAMURA<sup>5</sup>, AND NORIHISA ADACHI<sup>5</sup>

<sup>1</sup>Department of Virology, University of Toyama, <sup>2</sup>APS Japan Co., Ltd. <sup>3</sup>Shonan Ceramics Corporation, <sup>4</sup>Department of Metabolism, Diabetes and Nephrology, Fukushima Medical University Aizu Medical Center, <sup>5</sup>TechnoPLAS Japan Co., Ltd. Japan

Email: kshiraki@med.u-toyama.ac.jp

### **Abstract**

The efficiency of photocatalysis depends on the surface area and materials, and we have prepared a nanosized-titanium dioxide (TiO<sub>2</sub>)-coated ceramic irradiated by UV-LED lamps as a photocatalytic air cleaner. Ceramic filter system decomposed 80% of acetaldehyde and Particulate dioxins (40 pg/m<sup>3</sup>) and gaseous dioxins (16 pg/m<sup>3</sup>) were removed by 7.5 and 2.8 pg/m<sup>3</sup> by passing through four TiO<sub>2</sub>-coated ceramic (30 × 30 × 2 cm) under black-light, indicating about 80% of dioxin was decomposed by the photocatalysis. Ceramic was changed to aluminum plate and the efficiency was improved. The 90% of 5 ppm acetaldehyde (12.4 μmol/h) was decomposed and generated carbon dioxide (25.43 μmol/h; RC: 92.5% carbon dioxide conversion rate) efficiently and continuously for 200 min with the ratio of one acetaldehyde (12.40 μmol/h) to two carbon dioxide (25.43 μmol/h) at their molar ratios by being passed through the TiO<sub>2</sub>-coated aluminum plate (5x10x1 cm) under black light, indicating complete decomposition of acetaldehyde with high efficiency. This photocatalysis system was applied for elimination of acetaldehyde and inactivation of influenza aerosol in a closed cubic space using aluminum plates. Acetaldehyde at 20 ppm in a cubic 1 m<sup>3</sup> space was eliminated by 60 min at a half-life of 8 min. The aerosol-associated infectivity and the RNA genome of influenza virus produced by a nebulizer in a 779 liter cubic space were eliminated within 7 minutes but were detectable up to 28 minutes without the function of a photocatalytic air cleaner. Influenza virus was broken down by photocatalysis rather than being trapped by Hepafilter as intermediate breakdown products of influenza virus were observed. Thus, a photocatalytic air cleaner efficiently decomposed and eliminated organic chemicals, acetaldehyde, and aerosol-associated influenza virus infectivity and viral RNA, indicating a photocatalytic air cleaner functioned in the cleaning and detoxification of the air in the closed space for maintaining a safer environment.

**Kimiyasu Shiraki, MD, PhD**  
Professor and Chairman  
Department of Virology  
University of Toyama  
2630 Sugtani, Toyama 930-0194, Japan  
kshiraki@med.u-toyama.ac.jp



He graduated School of Medicine in 1977 and awarded PhD in 1983 at Osaka University and awarded Incentive Award from Isukura Memorial Foundation (1993), Incentive Award from Medical and Pharmaceutical Society (1994), Toyama Shinbun (Newspaper) Culture Award (2015), and Society award from Medical and Pharmaceutical Society (2016).

Professor and Chairman of the Department of Virology at the University of Toyama. Dr. Shiraki is interested in viral pathogenesis of influenza and herpesvirus. He has developed anti-influenza drug, Favipiravir, with Toyama Chemical Co., Ltd. and a new anti-herpesvirus drug Amenamevir. Favipiravir was used for treatment of Ebola virus infection in West Africa in 2014-2015. Amenamevir is a novel viral helicase-primase inhibitor and will open a new era of anti-herpetic therapy by its novel antiviral activity and better compliance than current anti-herpetic drugs. Dr. Shiraki is interested in the action of photocatalytic activity against aerosol influenza virus and utilized it as a photocatalytic air cleaner in the cleaning and detoxification of the indoor air in the closed space for maintaining a safer environment.

For more information, please visit [http://evaweb.u-toyama.ac.jp/html/661\\_en.html](http://evaweb.u-toyama.ac.jp/html/661_en.html).

**Session B5**

**B20**

**8:25 - 8:50 AM Room B June 21**

## Custom-engineered ZnO nanorods and ZnO nanodisks exhibit antibacterial effect towards *Bacillus subtilis* by damaging bacterial cell wall

Soh Fanny Chiat Orou<sup>1</sup>ξ, Kee Jeik Hang<sup>1</sup>ξ, Myo Thuya Thien<sup>2</sup>ξ, Ying Yuet Lee<sup>2</sup>ξ, Le Cheng Foh<sup>3</sup>, Nguyen Duong Ngoc Diem<sup>1</sup>, Goh Boon Hee<sup>1</sup>, Pung Swee Yong<sup>2\*</sup> and Pung Yuh Fen<sup>1\*</sup>

ξ all the four authors contributed equally

<sup>1</sup>Department of Biomedical Sciences, University of Nottingham (Malaysia campus), Semenyih, 43500 Selangor, Malaysia;

<sup>2</sup>School of Materials and Mineral Resources Engineering, Engineering Campus, Nibong Tebal, 14300 Penang, Malaysia;

<sup>3</sup>School of Bioscience, University of Nottingham (Malaysia campus), Semenyih, 43500 Selangor, Malaysia

Email: [sypung@usm.my](mailto:sypung@usm.my)

### Abstract

Metal oxide nanoparticles are versatile platforms for various biomedical, industrial, agricultural and environmental applications. In the recent decades, many studies have been focused on the emergence of metal oxide nanoparticles as photocatalysts. These relatively cheap and stable nanoscale photocatalysts possess good degradation effect on organic pollutants and potent bactericidal activities. However, the complex mechanisms of bactericidal activities by metal oxide nanoparticles are still controversial. Thus, this study aimed to investigate the antibacterial activity of custom-engineered ZnO nanorods and ZnO nanodisks, as compared to the commercially-available TiO<sub>2</sub> nanoparticles. Antibacterial susceptibility assay was carried out on *Bacillus subtilis* and *Staphylococcus aureus* (gram positive bacteria), and *Escherichia coli* and *Pseudomonas aeruginosa* (gram negative bacteria). While ZnO nanorods and ZnO nanodisks showed potent inhibition on *B. subtilis* and *S. aureus* with minimal inhibitory concentrations of 128 and 256 ug/ml respectively, no inhibition was found on gram negative bacteria. Since *B. subtilis* was a better model for gram positive bacteria, subsequent studies were carried out on *B. subtilis*. During the time-kill kinetics assay, the inhibitory effect of both ZnO nanorods and ZnO nanodisks were seen to be significant after t=90 min (\*  $p < 0.05$ ; n=2 to 3). To further elucidate the underlying mechanism(s), Rhodamine dye degradation assay as marker for reactive oxygen species generation was performed. Significant discoloration of dye was observed for both TiO<sub>2</sub> nanoparticles and ZnO nanorods as compared to ZnO nanodisks (\*  $p < 0.05$ ; n=3). Zeta potential assay showed that ZnO nanorods were positively charged at pH7; whereas ZnO nanodisks were negatively charged. Electron micrographs showed that the cell wall of *B. subtilis* treated with ZnO nanorods and ZnO nanodisks was compromised, leading to the leakage of the intracellular contents and cell death. Our results indicated that the antibacterial effects of ZnO nanorods and ZnO nanodisks appeared to be mediated through multiple chemical and physical properties of NPs. These multiple chemical and physical properties of NPs collectively contributing to nanotoxicity threshold required for bacterial inactivation. Hopefully, our

study will shed light on the complexity of the antibacterial properties of metal oxide nanoparticles, in order to avoid any safety issues that might arise with metal oxide nanoparticles usage in potable water, either in direct or indirect ways.

**Swee-Yong, Pung** is Assoc. Professor from School of Materials and Mineral Resources Engineering, Universiti Sains Malaysia, Malaysia. He received his PhD in Material Engineering and Materials Design from University of Nottingham, United Kingdom in 2010. His current research interests include Engineering of nanomaterials particularly ZnO, semiconductor photocatalysts and phosphor materials. His research has been carried out with significant output in terms of publications, innovation and grant awards.



For more information, please visit <http://material.eng.usm.my/index.php/ms/our-staff/academic/associate-professors>.



**Session B5**

**B21**

**8:50 - 9:15 AM Room B June 21**

## Nanostructured TiO<sub>2</sub> with oxygen vacancies for the decomposition of organics

CHIAKI TERASHIMA

Photocatalysis International Research Center, Research Institute for Science & Technology,

Tokyo University of Science

2641 Yamazaki, Noda, Chiba 278-8510, Japan

Email: terashima@rs.tus.ac.jp

### **Abstract**

Titanium dioxide (TiO<sub>2</sub>) has been widely not only studied but also applied in industrial fields as photocatalyst because of its environmentally and economically advantages with high chemical stability, earth abundant and bio compatible properties. However, its large band-gap for the activity to only UV light region, and the high recombination rate of photogenerated electron and hole pairs have to be overcome to utilize effectively sunlight and to enhance the photocatalytic performance. Recent enormous efforts to overcome the above-mentioned drawbacks have resulted in the one-dimensional TiO<sub>2</sub> nanotubes, nanofibers and nanorods to suppress the carrier recombination, and/or the heterojunction structure of TiO<sub>2</sub> with another semiconductor to achieve larger separation of the photogenerated electron and hole, as well as the modification of TiO<sub>2</sub> nanoparticles with gold clusters to expand the light conversion from UV to visible and near-infrared region. Here, we report simple and effective modification of nano-sized TiO<sub>2</sub> materials by in-liquid plasma processing, which is a non-thermal plasma discharged in liquid. The present study focused to treat pristine TiO<sub>2</sub> nanoparticles by the discharge in water-based solution and to investigate the material properties as well as the photocatalytic activities for decomposing organics. As a result of plasma treatment, we found the incorporation of oxygen vacancies on the sub-surface of TiO<sub>2</sub> nanoparticles, and concluded that the origin of photocatalytic enhancement for acetaldehyde decomposition under fluorescent lamp attributed in the recombination suppression by the surface trap of oxygen vacancies near the nanoparticles surface.

**Chiaki Terashima** was born in 1969 in Kanazawa, Ishikawa Prefecture, Japan. He received his Ph.D. degree (2003) in electrochemical analysis at Tokyo University under the supervision of Professor Akira Fujishima and Professor Kazuhito Hashimoto. His academic career started at Nagoya University as an associate professor (2010-2011) in Professor Osamu Takai's group, and then moved to Tokyo University of Science in 2012. He is currently an associate professor at Photocatalysis International Research Center, Tokyo University of Science. His research interests are focused on photoelectrochemistry, diamond electrochemistry, and plasma processing in liquid.



For more information, please visit <http://www.rs.tus.ac.jp/pirc/en/member/index.html>.

**Session B5**

**B22**

**9:15 - 9:40 AM Room B June 21**

## TiO<sub>2</sub>-C hybrid aerogel photocatalysts for methylene blue degradation

XIA SHAO, RUI ZHANG\*

Shanghai Institute of Technology

100 Haiquan Road, Shanghai, China

Email: zhangrui@sit.edu.cn, shaoxia@sit.edu.cn

### **Abstract**

TiO<sub>2</sub>-C hybrid aerogels were prepared by one-pot sol-gel process in ethanol, followed by supercritical drying and carbonization, using TiCl<sub>4</sub> as TiO<sub>2</sub> precursor, resorcinol-furfural as carbon precursors, ethyl acetoacetate (EA) as a chelating agent and propylene epoxide (PO) as a gel initiator. Ce doping was performed by adding cerous nitrate into the solutions that form gels to modify the photocatalytic properties. Microstructures of samples were characterized by XRD, SEM, TEM, UV-Vis, Raman spectroscopy, nitrogen adsorption, mercury porosimetry, XPS and IR spectroscopy and the photocatalytic properties for methylene blue degradation were tested under UV and Vis light irradiation. Results showed that the porous textures of the hybrid aerogels were related to TiCl<sub>4</sub>/resorcinol-furfural mass ratio, the molar ratios of EA/Ti and PO/Ti. The samples had large specific surface areas, high adsorption capacities for methylene blue, uniform distribution of TiO<sub>2</sub> nanoparticles as anatase in the amorphous carbon structure. The presence of the amorphous carbon inhibited both the growth of TiO<sub>2</sub> nanoparticles and their conversion from anatase to rutile phase. The adsorption of methylene blue followed the pseudo-second-order kinetics model and its degradation followed the first-order kinetics model. The maximum photocatalytic activity for methylene degradation was up to 4.23 times that of P25 for the TiO<sub>2</sub>-C hybrid aerogels carbonized at 800 °C. A partial reduction of Ti<sup>4+</sup> to Ti<sup>3+</sup> was found for the samples carbonized at 900 °C, which improved significantly the catalytic activity under visible light. Methylene blue can be degraded under visible light within 60 min with the Ce-doped TiO<sub>2</sub>-C hybrid aerogels or the undoped one carbonized at 900 °C. Adsorption coupled with photo excitement, reduced recombination rate of e/h pair, band gap narrowing by interaction of carbon with TiO<sub>2</sub>, partial reduction of Ti<sup>4+</sup> to Ti<sup>3+</sup> during carbonization or Ce-doping, and the increased light utilization via scattering by macropores are responsible for the improved catalytic performance as compared with P25 photocatalyst from Degussa.

**Rui Zhang** is Professor of Materials Sciences and Engineering. He is a Member of America Ceramic Society and America Chemical Society, an editorial board member of New Carbon Materials.

His current research interests include nanoporous materials, nanocomposites, filters and catalysts

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<http://materials.sit.edu.cn/s/27/t/156/7a/01/info31233.htm>.



Session B5

B23

9:40 - 10:05 AM Room B June 21

## Highly efficient visible-light-driven BiVO<sub>4</sub>-based Photoelectrode

### Materials

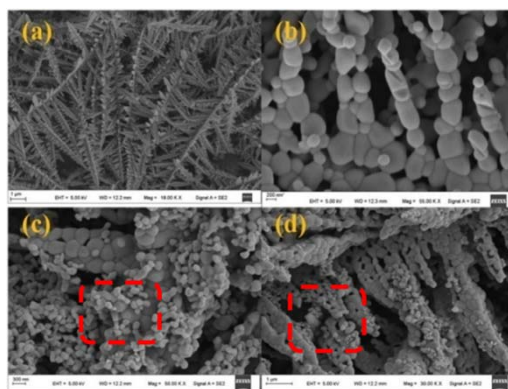
TENGJIAO NIU, JIJUAN HE, QIZHAO WANG\*

College of Chemistry and Chemical Engineering, Northwest Normal University  
Lanzhou, China

Email: wangqizhao@163.com, qizhaosjtu@gmail.com

### Abstract

BiVO<sub>4</sub> is an excellent visible-light-driven photocatalyst that can split water into O<sub>2</sub> for its more positive valence band than that of O<sub>2</sub>/H<sub>2</sub>O, whereas its positive conduction band makes it difficult to directly generate H<sub>2</sub> from H<sub>2</sub>O. But using the PEC, BiVO<sub>4</sub> can become a promising candidate as photoanode for hydrogen evolution performance. In our group, the leaf-like structure BiVO<sub>4</sub> photoelectrodes were prepared by electrochemical deposition, in which Zn<sup>2+</sup> ions were introduced as a direct agent to control the morphology and size of Bi nanoparticles [1]. NiFe<sub>2</sub>O<sub>4</sub> and CoFe<sub>2</sub>O<sub>4</sub> nanoparticles were loading on the surface of BiVO<sub>4</sub> to construct heterojunction. The heterojunctions can effectively prevent carriers from recombining and accelerate the separation of electrons and holes[2]. Besides, Bi/ BiVO<sub>4</sub>[3] and FeF<sub>2</sub>/ BiVO<sub>4</sub> can enhanced PEC hydrogen evolution performance.



**Fig.1** The SEM images of (a) as-obtained Bi in high concentration electrolyte; (b) BiVO<sub>4</sub> from the fruticose dracaena leaf structure Bi precursor film; (c) NiFe<sub>2</sub>O<sub>4</sub>/BiVO<sub>4</sub> electrode; (d) CoFe<sub>2</sub>O<sub>4</sub>/BiVO<sub>4</sub> electrode.

**References**

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- [3] Q.Z Wang, J.J He, Y.B. Shi, S.L. Zhang, T.J. Niu, H.D. She, Y.P. Bi. *Chem. Eng. J.*, 2017, DOI: 10.1016/j.cej.2017.05.171.

**Qizhao Wang** is an Associate Professor in the College of Chemistry and Chemical Engineering at the Northwest Normal University.

Dr. Wang's current research focuses on the design and synthesis of photocatalytic materials for various applications, with a focus on energy and environmental engineering. Dr. Wang has published more than thirty peer-reviewed journal articles and has been selected to the Program for the Young Innovative Talents of Longyuan by Gansu Province. Besides, he has received a number of prestigious awards, including the Ming De Outstanding Teacher Award and others.



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**Session B6**

**B24**

**10:20 - 10:45 AM Room B June 21**

## Highly Concentrated CO Evolution for Photocatalytic Conversion of CO<sub>2</sub> by H<sub>2</sub>O as an Electron Donor

KENTARO TERAMURA<sup>1,2,\*</sup>, KAZUTAKA HORI<sup>1</sup>, YOSUKE TERAOKA<sup>1</sup>, HIROYUKI TATSUMI<sup>1</sup>, ZEAI HUANG<sup>1</sup>, SHOJI IGUCHI<sup>1</sup>, ZHENG WANG<sup>1</sup>, HIROYUKI ASAKURA<sup>1,2</sup>, SABURO HOSOKAWA<sup>1,2</sup>, TSUNEHIRO TANAKA<sup>1,2,\*</sup>

<sup>1</sup>Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Kyotodaigaku Katsura, Nishikyo-ku, Kyoto 615-8510, Japan

<sup>2</sup>Elements Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University, Kyotodaigaku Katsura, Nishikyo-ku, Kyoto 615-8520, Japan

Email:teramura@moleng.kyoto-u.ac.jp

### Abstract

The reduction in human-induced emissions of CO<sub>2</sub> from automobiles, factories, power stations etc., over the next 15 years is currently one of the most important issues facing the planet. We should therefore attempt to develop industrial processes using CO<sub>2</sub> as a feedstock in order to build a sustainable society in the near future. Linear CO<sub>2</sub> molecules adsorbed on the surface of the solid bases are converted into unique structures, such as bicarbonate and carbonate species possessing lattice oxygen atoms. We believe that the process involves the capture and distortion of CO<sub>2</sub> upon adsorption on a solid base through activation by photoirradiation. Unstable CO<sub>2</sub> species adsorbed onto the surface can then be reduced by electrons with protons derived from H<sub>2</sub>O ( $\text{CO}_2 + 2\text{e}^- + 2\text{H}^+ \rightarrow \text{CO} + \text{H}_2\text{O}$ ). These days, we succeeded in designing highly selective photocatalytic conversion of CO<sub>2</sub> by H<sub>2</sub>O as the electron donor, by the simultaneous use of an inhibitor of the production of H<sub>2</sub> and a material for CO<sub>2</sub> capture and storage, such as ZnGa<sub>2</sub>O<sub>4</sub>/Ga<sub>2</sub>O<sub>3</sub><sup>[1]</sup>, La<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub><sup>[2]</sup>, SrO/Ta<sub>2</sub>O<sub>5</sub><sup>[3]</sup>, ZnGa<sub>2</sub>O<sub>4</sub><sup>[4]</sup> and ZnTa<sub>2</sub>O<sub>6</sub><sup>[5]</sup>, and Sr<sub>2</sub>KTa<sub>5</sub>O<sub>15</sub><sup>[6]</sup> with the modification of Ag cocatalyst. An isotope experiment using <sup>13</sup>CO<sub>2</sub> and mass spectrometry clarified that the carbon source of the evolved CO is not the residual carbon species on the photocatalyst surface, but the CO<sub>2</sub> introduced in the gas phase. In addition, stoichiometric amounts of O<sub>2</sub> evolved were generated together with CO.



## References

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**Kentaro Teramura** is currently an associate professor in Graduate School of Engineering of Kyoto University. He belongs to Department of Molecular Engineering. He was born in Kyoto, Japan. He studied at Kyoto University for both his undergraduate and graduate degrees. His doctoral thesis was in photoactivation of small molecules such as O<sub>2</sub>, NH<sub>3</sub>, and CO<sub>2</sub> adsorbed on various solid state materials under the direction of Professor Tsunehiro Tanaka and Professor Emeritus Takuzo Funabiki. After earning the Ph.D degree in engineering in 2004, he joined Department of Chemical System Engineering, Graduate School of Engineering, the University of Tokyo, where he worked as a postdoctoral fellow for 1 year and an assistant professor for 2 years under the leadership of Professor Kazunari Domen. Afterward he went back to Kyoto University in 2006 and contributed to Kyoto University Pioneering Research Unit for Next Generation (KUPRU) as a tenure-track assistant professor. He obtained a tenured lecturer position of Kyoto University in 2011 since he passed an intermediate screening at A rank and the final review at S rank at KUPRU. In 2011, he was selected as a researcher of Precursory Research for Embryonic Science and Technology (PRESTO), Science and Technology Agency (JST) and had a good opportunity to focus on artificial photosynthesis such as photocatalytic conversion of CO<sub>2</sub> by H<sub>2</sub>O. He promoted as an associate professor of Kyoto University in 2013. He won “The Japan Petroleum Institute Award for Encouragement of Research and Development” in 2012 and “The Catalysis Society of Japan Award for Encouragement of Research and Development” in 2013. Subject areas of his current interest include heterogeneous catalysis and photocatalysis, with emphasis on CO<sub>2</sub> capture and utilization (CCU). His motto is creating new science and unveiling a thing we don’t know. He has published more than 130 research papers, several patents, books and many book chapters.



**Session B6**

**B25**

**10:45 - 11:10 AM Room B June 21**

## Efficient Nanocatalysts for Solar-Energy-Driven Photocatalytic CO<sub>2</sub>

### Reduction

YUN-XIANG PAN

School of Chemistry and Chemical Engineering, Hefei University of Technology

E-mail: tjupyx@hfut.edu.cn

#### **Abstract**

Solar-energy-driven photocatalytic CO<sub>2</sub> reduction into valuable chemicals or fuels, such as CO and CH<sub>3</sub>OH, is a promising strategy for CO<sub>2</sub> capture and utilization. We have been focusing our research on developing efficient nanocatalysts for the photocatalytic CO<sub>2</sub> reduction. Firstly, we synthesized a biofilm, with a thickness of about 1.5 nm, from cold-plasma-assisted peptide self-assembly, for the photocatalytic CO<sub>2</sub> reduction to CO [1,2]. The biofilm-based nanocatalyst exhibits an enhanced CO evolution rate (19.4 μmol/h), as compared with the nanocatalyst without biofilm (2.8 μmol/h). This results from the unique flexibility of the biofilm for more efficient transfer of the photogenerated electrons. Secondly, we fabricated a Pt/Ga<sub>2</sub>O<sub>3</sub> nanocatalyst with abundant oxygen vacancies (V<sub>o</sub>) for the photocatalytic CO<sub>2</sub> reduction to CO [3,4]. The V<sub>o</sub> leads to more efficient CO<sub>2</sub> adsorption and separation of the photogenerated electron-hole pairs, and thereby enhanced CO production on V<sub>o</sub>-rich Pt/Ga<sub>2</sub>O<sub>3</sub> (21.0 μmol/h), as compared with the V<sub>o</sub>-poor Pt/Ga<sub>2</sub>O<sub>3</sub> (3.9 μmol/h). Thirdly, we found that In<sub>2</sub>O<sub>3</sub> nanobelts coated by a 5-nm-thick carbon layer provide an enhanced photocatalytic CO<sub>2</sub> reduction to CO and CH<sub>4</sub>, yielding CO and CH<sub>4</sub> evolution rates of 126.6 and 27.9 μmol/h, respectively, with Pt as co-catalyst [5]. The carbon coat promotes visible light absorption, electron-hole separation, CO<sub>2</sub> chemisorption, production of protons for reducing CO<sub>2</sub>, and thereby facilitates the CO and CH<sub>4</sub> production.

## **References**

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**Yun-Xiang Pan** is now a Distinguished Professor in School of Chemistry and Chemical Engineering at Hefei University of Technology of China. He received his PhD degree in Chemical Engineering from Tianjin University of China in 2010. From Jan. 2008 to Sep. 2009, he studied as a joint-training PhD student in Southern Illinois University Carbondale and Pacific Northwest National Lab in USA. After getting his PhD degree, he worked as a research fellow in Aarhus University of Denmark from Apr. 2010 to Apr. 2011, and in Nanyang Technological University of Singapore from Feb. 2013 to Sep. 2014. His research interest is the fabrication of catalysts for CO<sub>2</sub> conversion. He, as the first or corresponding author, has published more than 20 papers in international journals like *Journal of the American Chemical Society*, *Energy & Environmental Science*, *ACS Nano*, *Journal of Catalysis*, *Nano Research*, *ACS Applied Materials & Interfaces*, *ACS Sustainable Chemistry & Engineering*, *ChemSusChem*, *Journal of Power Sources*, *Chemistry-A European Journal*, *Journal of Physical Chemistry C*, *Langmuir* and *Catalysis Today*. He has co-authored other 20 papers in international journals including *Science*.



Session B6

B26

11:10 - 11:35 AM Room B June 21

## New Heterogeneous Photocatalysts Designed for Water Oxidation and CO<sub>2</sub> Reduction

KAZUHIKO MAEDA

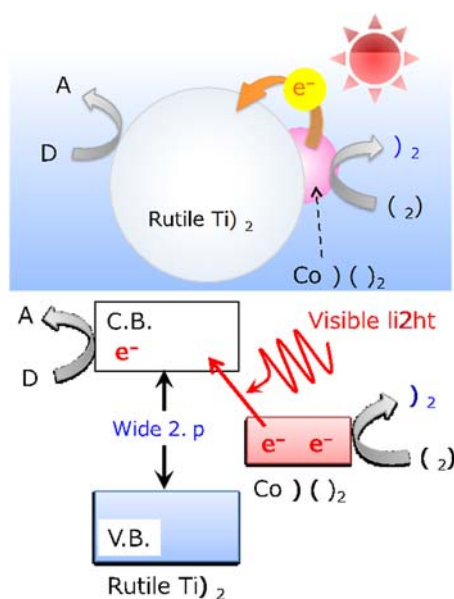
School of Science, Tokyo Institute of Technology

2-12-1-NE-2 Ookayama, Meguro-ku, Tokyo

Email: maedak@chem.titech.ac.jp

### Abstract

Water splitting and CO<sub>2</sub> fixation on heterogeneous photocatalysts are important reactions from the viewpoint of solar-to-fuel energy conversion. To achieve these reactions, it is important to improve both bulk and surface properties of a photocatalyst so as to suppress electron-hole recombination and promote surface redox catalysis. In this presentation, recent progress on the development of new photocatalysts that are active for such artificial photosynthetic reactions will be given. In particular, surface modification techniques developed by our group to construct active sites and light-absorbing centers will be presented. For example, we developed a new powdered photocatalyst consisting of Co(OH)<sub>2</sub> and TiO<sub>2</sub> [1]. It is well known that TiO<sub>2</sub> is an active photocatalyst, but only works under UV irradiation. By contrast, the Co(OH)<sub>2</sub>/TiO<sub>2</sub> hybrid photocatalyst is capable of absorbing visible light with wavelengths of up to 850 nm and oxidizing water into oxygen gas, even though it consists of only earth-abundant elements only. To our knowledge, this system provides the first demonstration of a photocatalytic material capable of water oxidation upon excitation by visible light up to such a long wavelength.



**Fig.1** Visible-light-driven water oxidation using Co(OH)<sub>2</sub>-modified rutile TiO<sub>2</sub>.

**References**

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**Kazuhiko Maeda** received his PhD from The University of Tokyo (2007) under the supervision of Professor Kazunari Domen. During 2008–2009, he was a postdoctoral fellow at The Pennsylvania State University, where he worked with Professor Thomas E. Mallouk. He then joined The University of Tokyo as an Assistant Professor in 2009. Moving to Tokyo Institute of Technology in 2012, he was promoted to an Associate Professor. He was also appointed as a PRESTO/JST researcher during 2010–2014. His major research interest is heterogeneous photocatalysis for light to chemical energy conversion, with a focus on water splitting and CO<sub>2</sub> fixation.





**Session B6**

**B27**

**11:35 - 12:00 PM Room B June 21**

## Facile Development of Nanostructured Photocatalysts for CO<sub>2</sub> Capture and Conversion

WEI-NING WANG

Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University

800 E. Leigh St., Richmond, Virginia, United States of America

Email: wnwang@vcu.edu

### **Abstract**

The continuous reliance on fossil fuel-based energy is inevitable. Rational strategies to reduce carbon dioxide (CO<sub>2</sub>) emissions are thus highly demanded. Developing efficient photocatalysts that can harness solar energy appears to be a promising methodology to capture and recycle CO<sub>2</sub> as a fuel feedstock. The conversion efficiency of the current photocatalysts, however, is generally very low due to various limiting factors, such as fast electron-hole recombination rates, narrow light absorption range, and backward reactions. Thus, developing strategies to overcome the above limitations is an important task in this field.

Here we present several strategies through controlled synthesis to address the aforementioned limitations toward enhancing the overall CO<sub>2</sub> conversion efficiency. Examples of novel photocatalysts being explored include mesoporous nanocomposite particles (i.e., Cu-TiO<sub>2</sub>-SiO<sub>2</sub>), [1,2] 1D structured Pt-TiO<sub>2</sub> thin films, [3] CuO-ZnO heterojunction nanowires, [4] and crumpled graphene-based nanoballs. [5,6] Systematic materials characterization and photocatalysis analysis of the materials, by electron microscopy, X-ray diffraction, gas chromatography, X-ray photoelectron spectroscopy, *in-situ* diffuse reflectance infrared Fourier transform spectroscopy, and femtosecond time-resolved transient absorption spectroscopy, aid in understanding the quantitative CO<sub>2</sub> photoreduction pathways and the correlations between materials properties and CO<sub>2</sub> photoreduction performance.

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**Wei-Ning Wang** is currently Assistant Professor in the Department of Mechanical and Nuclear Engineering at Virginia Commonwealth University (VCU). He received his B.E. (in Polymer Science and Engineering, 1999) and M.E. (in Materials Science and Engineering, 2002) from Nanjing Tech University in China. He obtained his Ph.D. in Chemistry and Chemical Engineering in 2006 from Hiroshima University in Japan under the guidance of Prof. Kikuo Okuyama. He was then a JSPS Postdoctoral Fellow and Assistant Professor in the Department of Chemical Engineering at Hiroshima University. From 2009-2012, he was Postdoctoral Research Associate at Washington University in St. Louis (WUSTL) working with Prof. Pratim Biswas in the Department of Energy, Environmental and Chemical Engineering. He was then promoted to Research Assistant Professor at WUSTL prior to joining the faculty at VCU. His research mainly concerns advanced functional materials development via aerosol routes for energy and environmental applications. He has published over 80 peer-reviewed journal articles, 8 review papers, and 5 book chapters.



**Session B7**

**B28**

**14:00 - 14:25 PM Room B June 21**

## Low Dimensional Materials Used for Lithium / Sodium ion Battery Anode

GAOXIANG WU, XIAODAN LI, JIEWEI CHEN, YANJIAO GUO, BI LUO, BING JIANG, LIHUA CHU, MEICHENG LI\*

State Key Laboratory of Alternate Electrical Power System with Renewable Energy Sources, School of Renewable Energy, North China Electric Power University

Beinong Road 2, Beijing 102206, China

\*Email: mcli@ncepu.edu.cn; Tel: 15810669688.

### Abstract

The exploitation of high-performance lithium ion batteries is an effective way to promote the practicality of electric vehicles and the large scale development of renewable energy. We have designed and used a low temperature solution approach which is simple, low cost, scalable to synthesize  $Zn_2GeO_4/g-C_3N_4$  hybrid structure. Furthermore the synergistic effect on their lithium storage has been discussed. The  $Zn_2GeO_4/g-C_3N_4$  hybrids exhibited highly reversible capacity of  $1370 \text{ mA h g}^{-1}$  at  $200 \text{ mA g}^{-1}$  after 140 cycles and excellent rate capability of  $950 \text{ mA h g}^{-1}$  at  $2000 \text{ mA g}^{-1}$ . On the other hand, molybdenum sulfide, one of the transition metal sulfides, has been considered as a hopeful anode material, because of the small volume change ( $\sim 103\%$ ) and the high theoretical capacity ( $669\sim 1675 \text{ mA h g}^{-1}$ ). In order to improve the electrochemical properties of molybdenum sulfide, we have designed and prepared  $TiO_2@MoS_2$  core-shell structure. This composite structure provides a plenty of surface active sites for rapid transportation of lithium ions and orderly path for electrons. As a result, the electrochemical performance of  $TiO_2@MoS_2$  is much higher than that of molybdenum sulfide as well as titanium dioxide. In addition, transition metal oxides also have been attracted widespread attention, because of its versatile nanostructures, high theoretical capacity and small volume change. We have synthesized 3D NiO microsphere architecture assembled from porous nanosheets via easy hydrothermal method. The advantage of large specific surface area endows the as-prepared 3D NiO microspheres with a good performance of stable and high reversible discharge capacity up to  $820 \text{ mA h g}^{-1}$  even after 100 cycles at a current density of  $100 \text{ mA g}^{-1}$ , and good rate capability of  $634 \text{ mA h g}^{-1}$  at a high current density of  $1 \text{ A g}^{-1}$ .

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- Lihua Chu, Meicheng Li\*, Xiaodan Li, et. al. *RSC Advances*, 2015, 5, 49765 - 49770

**Meicheng Li** is Professor of Energy Materials and Devices and Director of the Center for New Energy Materials and Photoelectric Technology at School of Renewable Energy in North China Electric Power University. Till now, he contributed more than 180 journal articles and performed the review services for about 60 SCI journals. He got almost 10 items of awards for the science and technology success. He served several academic conferences as the chair, track co-chair or session chair. He is an executive fellow of the China Energy Society, fellow of Chinese Society for Optical Engineering, a member of the Materials Research Society, and senior member of Chinese Institute of Electronics.



His current research interests is New Energy Materials and Devices, focusing on the nanostructures of silicon, carbon and oxide etc., and the relative novel device applications in energy harvesting, conversion, and storage.

For more information, please visit <http://nemd.ncepu.edu.cn>

**Session B7**

**B29**

**14:25 - 14:50 PM Room B June 21**

## **Noble metal-free Metal Sulphides as Highly Efficient Visible Light Driven Photocatalysts for H<sub>2</sub> Production from H<sub>2</sub>S**

YING ZHOU, MENG DAN

[a] State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University

[b] The Center of New Energy Materials and Technology, School of Materials Science and Engineering, Southwest Petroleum University

Chengdu 610500, China

Email: yzhou@swpu.edu.cn, danmeng6868@163.com

ARVIND PRAKASH

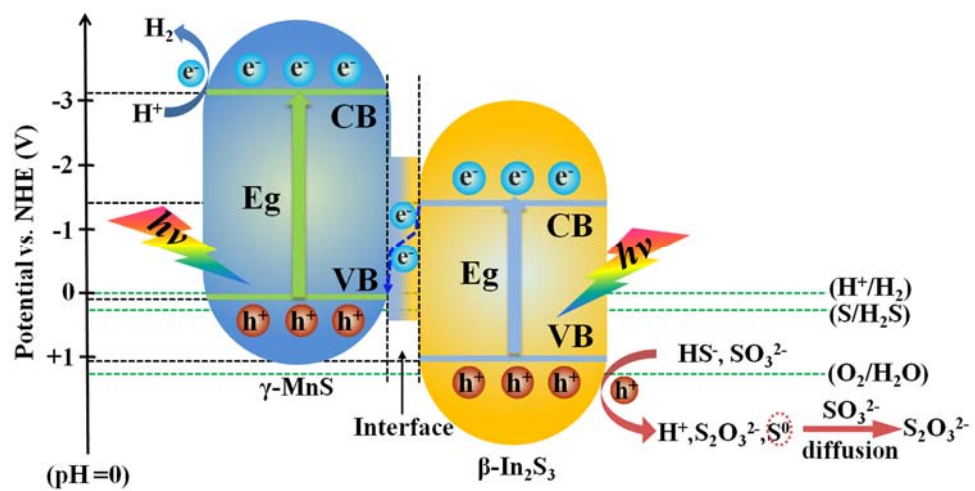
The Center of New Energy Materials and Technology, School of Materials Science and Engineering, Southwest Petroleum University

Chengdu 610500, China

Email: arvindprakash124@yahoo.com

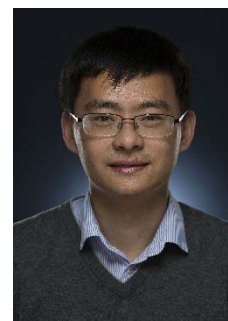
### **Abstract**

Hydrogen sulfide is an extremely toxic gas which is generated from both nature and human factors. Recently, photocatalytic splitting of H<sub>2</sub>S into H<sub>2</sub> and S has attracted great attention because hydrogen production and H<sub>2</sub>S removal are simultaneously achieved. However, the deactivation of the photocatalysts and lack of suitable setup for photocleavage of H<sub>2</sub>S to H<sub>2</sub> limit its wide application. Herein, we constructed a complete setup for H<sub>2</sub> production from H<sub>2</sub>S. This setup has some functions including H<sub>2</sub>S absorption, decomposition and product recovery. Simultaneously, a series of MnS/In<sub>2</sub>S<sub>3</sub> composites were successfully fabricated by a solvothermal method. A maximum H<sub>2</sub> production rate of 8360 μmol g<sup>-1</sup> h<sup>-1</sup> can be achieved over MnS/In<sub>2</sub>S<sub>3</sub>\_0.7 catalyst, and the corresponding QE of this sample is as high as 34.2% at 450 nm even in the absence of any noble-metal co-catalysts. Importantly, MnS/In<sub>2</sub>S<sub>3</sub> composite displays a good stability and also anti-photocorrosion. Additionally, in order to further enhance visible-light photocatalytic H<sub>2</sub> production activity of MnS/In<sub>2</sub>S<sub>3</sub>, MnS/In<sub>2</sub>S<sub>3</sub>/CuS composites were prepared through solvothermal treatment. And a maximum H<sub>2</sub> production rate of 29252 μmol g<sup>-1</sup> h<sup>-1</sup> can be achieved over a MnS/In<sub>2</sub>S<sub>3</sub>/CuS with optimized composition, which is 3.5 times higher than that of MnS/In<sub>2</sub>S<sub>3</sub>\_0.7, and this reveals that the addition of CuS can effectively increase the photocatalytic activity for splitting H<sub>2</sub>S into H<sub>2</sub>. All in all, suitable setup for photocatalytic splitting of H<sub>2</sub>S and noble-metal free metal sulphides photocatalysts have great significance for photocleavage of H<sub>2</sub>S to H<sub>2</sub>.



**Fig.1** Photocatalytic process of splitting  $H_2S$  in 0.6 M  $Na_2SO_3/0.1$  M  $Na_2S/3$  M  $H_2S$  solution

**Ying Zhou** is a professor of School of Materials Science and Engineering of Southwest Petroleum University, and a member of Royal Society of Chemistry and International Society of X-ray Absorption Fine Structure Spectroscopy. As a scholar, he was ever rewarded a Alexander von Humboldt Fellowship at Karlsruhe Institute of Technology with Prof. Jan-Dierk Grunwaldt.



In 2004, he graduated from the specialty of Inorganic Non-metal of Central South University. In 2007, he obtained master's degree of materials science in Shanghai Institute of Optics and Fine Mechanics. In 2010, he received PhD in University of Zurich in Switzerland (UZH), and continued his postdoctoral research with Outstanding Youth Fund of the University of Zurich for one year. Then he started to shoulder on teaching and science research in Southwest Petroleum University.

His current research interests include oil gas utilization, catalytic materials and in situ techniques on materials synthesis and action.

For more information, please visit <http://energy.swpu.edu.cn/english/group/1/1/19.html>



**Session B7**

**B30**

**14:50 - 15:15 PM Room B June 21**

## Photoelectrocatalytic Production of Solar Fuels from Water and CO<sub>2</sub>

HYUNWOONG PARK

School of Energy Engineering, Kyungpook National University

Daegu 41566, Republic of Korea

Email: hwp@knu.ac.kr

### Abstract

There is renewed interest in the photocatalytic and photoelectrochemical conversion of CO<sub>2</sub> into value-added chemicals using various semiconductor particles and electrodes. Common CO<sub>2</sub> reduction products are C1 chemicals (CO, HCOOH, CH<sub>3</sub>OH, and CH<sub>4</sub>) in aqueous media, while the production of C2-C4 hydrocarbons (e.g., C<sub>2</sub>H<sub>6</sub> and C<sub>3</sub>H<sub>8</sub>) has also been reported. A number of solar-active materials have been reported, but they still suffer from low selectivity, poor energy efficiency, and instability, while failing to drive simultaneous water oxidation. In this regard, p-type CuMO<sub>2</sub> (where M = Al<sup>3+</sup> and Fe<sup>3+</sup>) is highly promising because of its unique structure; suitable bandgap energies; high conduction band level, which is sufficient for H<sub>2</sub> production and CO<sub>2</sub> reduction; and relative stability in aqueous solution. Unfortunately, the typical synthetic route for CuMO<sub>2</sub> is annealing a Cu(I) and M(III) salt mixture at high temperature, which inevitably results in irregular, coarse particles of several micrometers. Furthermore, the as-synthesized particles are difficult to fabricate into durable films on transparent conducting oxide (TCO) substrates because of the absence of particle-to-particle interaction. Even if they are fabricated, the films have less intimate and looser interparticle connections undergoing a significant charge recombination at the solid/solid interface. This difficulty in synthesizing CuMO<sub>2</sub> films has caused this material to be less studied despite its potential as a promising photocathode. With this in mind, we have attempted to synthesize high-efficiency CuMO<sub>2</sub> films on TCO substrates via electrochemical deposition. This talk presents our recent studies on the solar CO<sub>2</sub> conversion to value-added chemicals while using water as an electron donor in various photo-systems [1-12].

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- [12] H. Park and W. Choi, *Energy & Environmental Science* 9 (2016) 411 (*Cover paper*).

**Prof. Hyunwoong Park** received a B.S. in Environmental Science at Hallym University (Chuncheon, Korea) in 1999 and a Ph. D degree in Environmental Engineering at POSTECH (Pohang, Korea) in 2004. After postdoctoral research at Caltech (Pasadena, California), he joined the faculty of School of Energy Engineering, Kyungpook National University (Daegu, Korea) as an assistant professor (2008) and was promoted to associate professor (2012). His primary research interests are focused on artificial photosynthesis and electrocatalysis. He has published over 120 papers in peer-reviewed journals, which have been cited over 6600 times (H-index 43). He is serving as an Editor of Materials Science in Semiconductor Processing (Elsevier, 2015–Present).



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**Session B7**

**B31**

**15:15 - 15:40 PM Room B June 21**

## Significant photocatalytic enhancement via strengthening interface with TiO<sub>2</sub> by carboxyl-functionalized conjugated polymers

YI DAN

State Key Laboratory of Polymer Materials Engineering of China (Sichuan University), Polymer Research Institute of Sichuan University, Chengdu 610065, China

Email: danyichenweiwei@163.com

### **Abstract**

Strengthening the interface between conjugated polymers and TiO<sub>2</sub>, where electron transfer happens, is of vital importance for the photocatalytic efficiency of conjugated polymer/TiO<sub>2</sub> hybrids, who may offer a promising future for photocatalysts. In this work, carboxyl-functionalized P3HT was synthesized via a simple oxidative copolymerization of 3-hexylthiophene and 3-thiophenic acid, which was subsequently bound to the surface of TiO<sub>2</sub>, resulting in an enhanced interface between them, demonstrated by the results of dissolution test. When the comonomer contains 15% 3-thiophenic acid, the visible light photocatalytic activity of P3HT/TiO<sub>2</sub> composites of carboxyl-functionalized polymers for degradation of methyl orange is 2.2 and 5.3 times as great as that of unfunctionalized polymer and TiO<sub>2</sub>, respectively. The significant enhancement of photocatalytic activity can be ascribed to the favored electron injection and facilitated separation of photogenerated carriers owing to the strengthened interfacial electronic coupling interaction between the carboxyl-functionalized P3HT and TiO<sub>2</sub> according to the results of PL spectra and trapping experiments. This may give a useful enlightenment for the preparation of more effective and practical conjugated polymer/TiO<sub>2</sub> photocatalysts.

**Keywords:** Composites, interfacial, photocatalytic, visible light, charge transport, poly(3-hexylthiophene), TiO<sub>2</sub>

**Yi Dan** is Professor of State Key Laboratory of Polymer Materials Engineering of China (Sichuan University) and Polymer Research Institute of Sichuan University. Her primary research Interests are (1) Polymer synthesis and modification by emulsion polymerization, controllable polymerization and blending/Synthesis of polylactide macro-initiator and polylactide-block-polymethyl methacrylate / Controllable radical polymerization of vinyl monomers and its application in modifying polymers; (2) Degradation rules of polymer materials, e.g., polylactide and polycarbonate, under environment factors, such as., ultraviolet irradiation, hot water, chemicals and atmosphere, and the stabilization of polymers; (3) Environmental friendly polymer materials, e.g., biodegradable PLA, polymer/TiO<sub>2</sub> composite photo-catalytic materials used for treating waste water and for cleaning air.



**Session B8**

**B32**

**16:00 - 16:25 PM Room B June 21**

## Ag nano-doping onto microsized TiO<sub>2</sub>: a challenge for enhancing the photocatalytic abatement of air pollution under visible light

G. CERRATO<sup>\*,1,4</sup>, C. BIANCHI<sup>2,4</sup>, M. STUCCHI<sup>2,4</sup>, V. CAPUCCI<sup>3</sup>

<sup>1</sup> Dept. of Chemistry, University of Torino, via P. Giuria, 7 – 10125 Torino (ITALY)

<sup>2</sup> Dept. of Chemistry, University of Milano, via Golgi, 19 – 20133 Milan, Italy

<sup>3</sup> GranitiFiandre SpA, via Radici Nord, 112 - 42014 Castellarano (RE), Italy

<sup>4</sup> INSTM Consortium, via G. Giusti, 9 - 50121 Firenze (ITALY)

Email: giuseppina.cerrato@unito.it

### Abstract

Surface modification of TiO<sub>2</sub> supports is one of the most exploited way to solve the problem of TiO<sub>2</sub> low activity under visible light. Ag metal nanoparticles (Ag-NPs) deposited onto microsized titania can positively impact on the photocatalytic activity towards volatile organic compounds (VOC) and NO<sub>x</sub> abatement even in the absence of UV-A. We employed a commercial micro-sized titania support (1077 by Kronos), formally sold as a pigment, even though titania nanopowders exhibit better photoactivity, because of the many drawbacks connected to the use of NPs, as these can be inhaled and come into direct contact with the cells of the organisms, leading to severe health damages [1]. We prepared samples with different Ag content to evaluate the impact of the amount on the photocatalytic performances, tested for the above mentioned molecules employing a LED lamp to avoid any UV light contribution. We found interesting correlations between the photocatalytic performances and size/shape of Ag-NPs, the latter features being investigated by means of several experimental techniques, such as HR-TE microscopy, X-Ray diffraction, FT-IR and UV-Vis spectroscopies, ICP-MS analysis, etc. [2] We also found that the synthetic route applied to deposit Ag-NPs plays an important role in defining the final photocatalytic performances.

### References

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- [2] C. L. Bianchi et al, *Trends in Photochemistry & Photobiology*, 17 (2016) 31-43, Copyright © 2016 Research Trends

**Giuseppina CERRATO** is Associate Professor of Inorganic Chemistry at the University of Turin (Italy). She is also affiliate to the Interdepartmental Nanostructure and Interfaces Centre (same University) and to the INSTM Consortium (Florence – Italy). She is a Member Società Chimica Italiana (SCI). G. Cerrato is co-author of ~130 papers published in major international journals (ISI, h index = 32: citations: 3324; May 2017) devoted to Inorganic and Physical Chemistry, Catalysis, Surface Science and Nanotechnology.



Her current research interests include the study of highly dispersed (nanostructured) oxidic systems, employed either in (i) heterogeneous catalysis/photocatalysis, or as (ii) structural ceramics, dental/prosthetic implants and/or supports for drug delivery systems.

For more information, please visit <http://www.chimica.unito.it/persona/giuseppina.cerrato>

## Session B8

B33

16:25 - 16:50 PM Room B June 21

## Functionalized graphene with both physical and chemical adsorptions of charges for high-performance supercapacitors

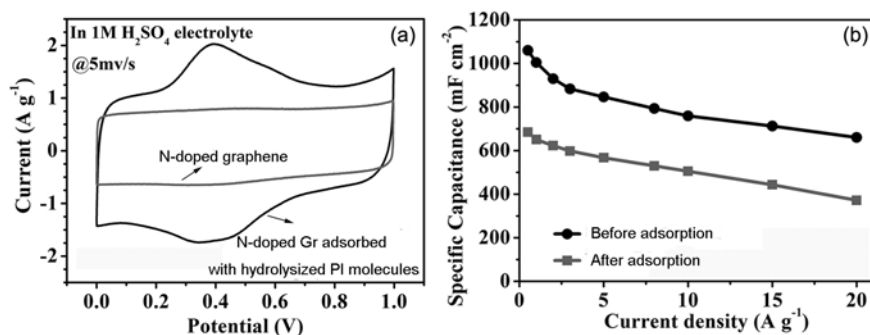
JINZHANG LIU, YI ZHAO

Beihang University, Beijing, 100191, China

Email: ljz78@buaa.edu.cn

**Abstract**

Carbon-based supercapacitor is also called electric double-layer capacitor that store energy via physical adsorption and desorption of ions from the electrolyte. Pseudocapacitors based on metal oxides or conductive polymers store energy via a redox process and generally have higher specific capacitance compared to the EDL type. Graphene has been regarded as an ideal candidate for supercapacitor applications, while the specific capacitance achieved so far in the lab, normally 200-300 F/g, is much lower than its theoretical value of 550 F/g. In order to enhance the charge storage capacity of graphene, we functionalized reduced graphene oxide by N-doping and adsorption of small molecules of hydrolyzed polyimide (PI). In N-doped graphene, the N-O bonds are responsible for the enhanced capacitance owing to their pseudo capacitive property [1]. Further, we found that the hydrolysis of PI can release small molecules into water solution, and these aromatic molecules adsorbed onto graphene via  $\pi$ - $\pi$  interaction have a significant effect in increasing the capacitance. With merely 3% weight increase after adsorption, the specific capacitance is about 40% increased. High capacitance over 420 F/g can be easily achieved from the functionalized graphene electrode in  $\text{H}_2\text{SO}_4$  aqueous electrolyte, even the electrode has high mass loading around  $5 \text{ mg/cm}^2$ . In  $\text{Li}_2\text{SO}_4$  aqueous electrolyte that can extend the operation voltage window to 1.6 V, the specific capacitance also remains high around 400 F.



**Fig.1** (a) Comparison to the electrochemical performance of N-doped graphene electrode before and after adsorption of hydrolyzed PI molecules. (a) CV curves. (b) Capacitance Vs. discharging current density in galvanostatic CD measurement.

**References**

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**Jinzhang Liu** is an Associated Professor of Materials Science and Engineering at Beihang University, Beijing, China. He received his PhD in Condensed Matter Physics from Lanzhou University, China in 2006, after which he worked in South Korea and Australia for academic research and joined Beihang University in Jan 2015. His current research interests include the preparation of carbon nanomaterials, dielectric materials, and electrochemical energy storage devices. He has authored about 50 research papers in the field of nanoscience and nanotechnology.



**Session B8**

**B34**

**16:50 - 17:15 PM Room B June 21**

## Enhanced Catalysis by Optical Nanoantenna Reduced on Transition Metal Dichalcogenide

DONALD KEITH ROPER<sup>A,B</sup>, JEREMY DUNKLIN<sup>B</sup>, ALEXANDER O'BRIEN<sup>B</sup>

<sup>A</sup>Microelectronics Photonics Graduate Program

<sup>B</sup>Ralph E Martin Department of Chemical Engineering (University of Arkansas)

NANO 206

731 W. Dickson St.

Fayetteville, AR 72701

Email: dkroper@uark.edu

### **Abstract**

Photocatalysis of hydrogen from water is limited by incomplete absorption of solar radiation and by uncontrolled disposition of generated carriers. Nanoantenna (NA)-induced coupling of photons to excitons could enhance photocatalytic solar fuel generation by increasing broadband optical absorption and by injecting energetic electrons where NA interfaces with semiconductor catalyst. This work examined catalysis of hydrogen evolution reaction (HER) by monolayer (1L) transition metal dichalcogenide (TMD) with and without decoration by optical NA. Spectroscopic and microscopic characterization of heterostructures of 1L-TMD and NA self-assembled via exfoliation and redox chemistry was compared with discrete dipole simulation. Electrodes inked with 1L tungsten disulfide (WS<sub>2</sub>) onto which NA was electrochemically reduced exhibited higher HER relative to 1L-WS<sub>2</sub> in neat or physically NA-decorated forms as measured by linear sweep and cyclic voltammetry. Coordinated simulation and measurement of supports improved design of 1L-TMD-NA photocatalysts and their implementation in chemical, biological, energy and water systems.

**Dr. Keith Roper** holds the Charles W. Oxford Professorship of Emerging Technologies in the Ralph E. Martin Department of Chemical Engineering at the University of Arkansas (UA). He served as Program Leader for the Engineering Research Centers and the Network for Computational Nanotechnology at the National Science Foundation (NSF) from 2014-2016. He is a Fellow of the American Institute for Medical and Biological Engineering and a member of the Arkansas Academy of Science. He is currently Associate Director of the Microelectronics Photonics Graduate Program at UA.



His research examines frameworks for innovation as well as advanced functionalities offered by active electrostatics to next-generation nano-, bio-, and meta-materials. His discoveries enable interactions between subatomic particles that are critical to information and energy flows in material and biological systems to be engineered in order to combat epidemic disease, accelerate secure information processing, and advance sustainable infrastructure. His research received recognition from EPA and DOE and has been featured by *SPIE Newsroom*, *NSF Discoveries*, *R&D Mag*, and over forty other media outlets. From 2012-2014, he was Program Director in the Education Engineering and Centers Division at NSF. He has held faculty appointments in chemical engineering, bioengineering and materials science and engineering at the University of Utah and the University of Arkansas. From 1994-2000 he developed processes for cell culture, fermentation, recovery, and analysis of protein, nucleic acid, bacterial polysaccharide, and adenoviral-vectored antigens at Merck & Co. He received a Ph.D. from the University of Wisconsin–Madison. He consults with university, industry, and government leaders to develop university-industry-government partnerships to translate discovery to marketable innovations as well as in biotechnology, biopharmaceuticals, chemicals, optoelectronics, and energy. He has authored or coauthored more than 79 technical articles and published proceedings, 71 invited lectures and 121 conference presentations, two textbooks, two book chapters, three U.S. patents, one E.P. patent, and six U.S. patent applications. He was instrumental in developing one viral and three bacterial vaccine products, sixteen Good Manufacturing Process documents, and multiple bioprocess equipment designs. He is active in ACS, AIChE, AIMBE, ASEE, IBE, SBE, SPIE, and Tau Beta Pi.

For more information, please visit <https://nbphotonics.uark.edu/>

**Session B8**

**B35**

**17:15 - 17:40 PM Room B June 21**

## Synergistic effect of MoS<sub>2</sub>/TiO<sub>2</sub> heterostructures with enhanced photo- and electro-catalytic performance

LIXIU GUAN,<sup>1</sup> GUIFENG CHEN,<sup>2</sup> XIAOLIN SONG,<sup>2</sup> HONG WANG,<sup>2</sup> AND JUNGUANG TAO,<sup>2,\*</sup>

<sup>1</sup>School of Science, Hebei University of Technology, Tianjin 300401, China

<sup>2</sup>Key Lab. for New Type of Functional Materials in Hebei Province, School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China

Email: jgtao@hebut.edu.cn

### **Abstract**

Herein, different MoS<sub>2</sub>/TiO<sub>2</sub> heterostructures are prepared with appropriate interface modifications. Electronic structure analysis shows that type II band alignments are realized at the interface, which efficiently drives the photo-excited charge to separate. Moreover, the band offsets can be delicately controlled by surface states with significant effect on their photocatalytic performance. In addition, the synergistic effect between MoS<sub>2</sub> and TiO<sub>2</sub> enhances the hydrogen evolution reaction (HER) activity of their hybrids which is tunable via interface engineering. The observed Tafel slop of 66.9 mV/dec for MoS<sub>2</sub>/TiO<sub>2</sub>-H complexes suggests the Volmer–Heyrovsky mechanism. The enhanced activities was attributed to the abundant active sites at the interfaces as well as the improved charge transfer efficiency.

**Junguang Tao** is Professor of Hebei University of Technology. He has authored 1 book chapter and ~40 journal papers. The total citation has reached over 900. H-index is 15. He is a reviewer for: *Phys. Rev. Lett., Nanoscale, Sci. Rep. Phys. Rev. B, Nanotechnology, Appl. Phys. Lett., J. Appl. Phys, etc.* Currently, he is the PI of several National and provincial level projects. His current research interests include engineering metal oxides for tuning their photocatalytic and photoelectric properties; preparation and hydrogen evolution reaction characterization of 2D transition metal dichalcogenides.



**Session A9**

**A39**

**8:00 - 8:25 AM Room A June 22**

## Terahertz filter and demultiplexer with photonic crystal waveguide

HONGJUN LIU, ZHAOLU WANG, NAN HUANG, JING HAN

State Key Laboratory of Transient Optics and Photonics Technology, Xi'an Institute of Optics and Precision Mechanics, Chinese Academy of Science

NO.17 Xinxu Road, New Industrial Park, Xi'an Hi-Tech Industrial Development Zone, Xi'an, Shaanxi, China

Email: liuhongjun@opt.ac.cn

### Abstract

Terahertz (THz) wave is finding growing applications in various important fields such as space science, communications, and security screening [1]. Besides sources and detectors, development of THz technologies also requires devices to guide and manipulate THz waves. The demand for high performance quasi optic components such as frequency filters, demultiplexer, attenuators, splitters, and polarizers is increasing [2]. We theoretically propose and investigate a magnetically tunable narrow-band terahertz filter and a multi-channel THz wavelength division demultiplexer based on photonic crystal waveguide. The optical properties of the filter have been analyzed in detail. It is found that a single resonant peak with the central frequency of  $\sim 1$  THz is existed in the transmission spectrum, which has a narrow full width at half maximum of  $< 2$  GHz. Moreover, under the control of an external magnetic field, transmission frequency and width of passband are adjustable, which reveals that the 2-D silicon photonic crystal waveguide with point and line defects can serve as a continuously tunable bandpass filter at the terahertz waveband. THz division demultiplexer consists of an input waveguide that perpendicularly coupled with a series of defects cavities, each of which captures the resonance frequency from the input waveguide. Coupled-mode theory and finite element method are used to analyze the transmission properties of the structure. It is found that the transmission wavelength centered around 1 THz can be adjusted by changing the geometrical parameters of defects cavities, which equals to THz waves generated by optical methods such as difference frequency generation and optical rectification.

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**Hongjun Liu** is Professor of Optics and Director of Optical Parametric Technology Group at the State Key Laboratory of Transient Optics and Photonics Technology, Xi'an Institute of Optics and Precision Mechanics, Chinese Academy of Sciences. He is the member of the Young Promotion Union of Science and Technology of Chinese Academy of Science, and the member of Photoelectronic Technology Professional Committee of Chinese Society of Astronautics, the member of China Optical Engineering Society. Until now, he has presided over the completion of more than 20 national research projects, and published more than 150 research papers.



His current research interests include the generation and amplification of ultrashort pulse, optical parametric amplification, optical nonlinear imaging technology, terahertz technology, fiber laser technology, silicon photonics technology and nonlinear optics.

**Session A9**

**A40**

**8:25 - 8:50 AM Room A June 22**

## **THz radiation based on fiber-integrated photo-conductive antennas and mode-locked Yb-doped fiber laser**

MIN YONG JEON\*, JI SU KIM, AND HYUN MOON YANG

Chungnam National University

99 Daehak-ro Yuseong-gu, Daejeon, 34134 Korea

\*Email: myjeon@cnu.ac.kr

SANG-PIL HAN, KIWON MOON, AND KYUNG HYUN PARK

Electronics and Telecommunications Research Institute (ETRI)

218 Kajong-ro Yuseong-gu, Daejeon, 34129 Korea

### **Abstract**

We present a THz radiation based on fiber-integrated photo-conductive antennas and a passively mode-locked Yb-doped fiber laser using a birefringent plate as a wavelength spectral filter. The mode-locked Yb-doped fiber laser is constructed with all-normal dispersion region using a single-mode optical fiber and a birefringent spectral filter. We characterize the outputs of the mode-locked Yb-doped fiber laser according to the azimuthal angle and optical axis of the birefringent spectral filter. The THz radiation is generated by injecting the pre-chirped optical pulses to the THz measurement system, which is constructed using two fiber integrated log-spiral-based low-temperature-grown (LTG) InGaAs photo-conductive antenna modules. We achieve over 2.5 THz spectral bandwidth and measure the various absorption lines of the water vapor in the free space.



**Min Yong Jeon** received the B.S. degree from Han Yang University, Seoul, Korea, in 1988, and the M.S. and Ph.D. degrees from Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea, in 1990 and 1994, respectively, all in physics. He has been with the Chungnam National University, Daejeon, Korea as a Professor of physics since May 2003. Prior to joining Chung Nam University, he worked in the area of optical router, as a Research Scientist at the University of California, Davis. From 1994 to 2001, he worked in the area of the optical network subsystem at the Electronics and Telecommunications Research Institute (ETRI), Daejeon, Korea. His current research focuses on optical coherence tomography, wavelength-swept lasers, optical fiber sensors, and optical terahertz wave generation.



## Session A9

A41

8:50 - 9:15 AM Room A June 22

## Generation and Detection of Terahertz Radiation from Laser-Plasmas

XIAO-YU PENG, HAI-WEI DU

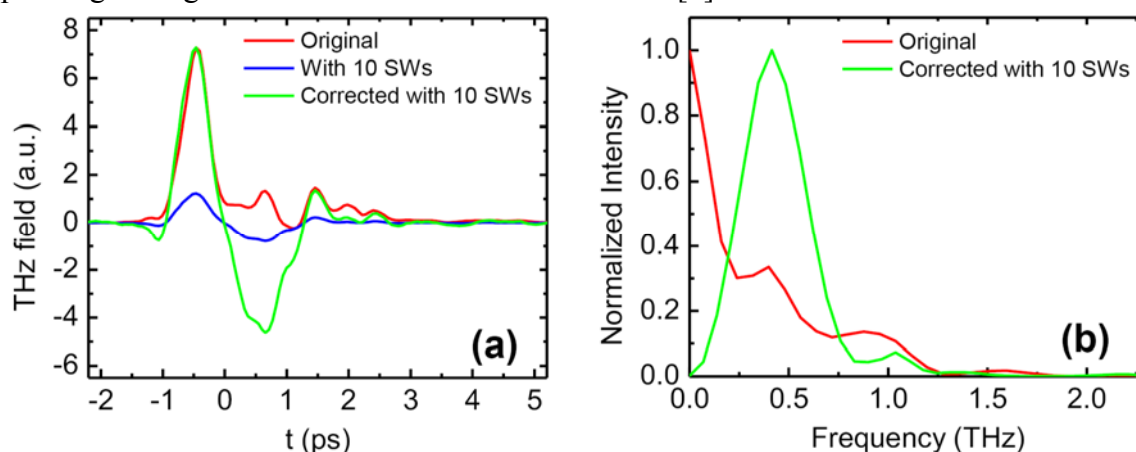
Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Sciences

No. 266 Fangzheng Avenue, Beibei District, Chongqing, China

Email: xypeng@cigit.ac.cn

**Abstract**

Broadband terahertz (THz) radiation from laser-plasma interaction and a corresponding broadband THz time domain spectroscopy based on optically-air-biased-coherent-detection technique are presented. One of the single-shot detection techniques for THz time domain spectroscopy, the spectral-encoding technique, is also reviewed [1]. Distortions of the signals measured by this technique and the corresponding strategies to reduce them are demonstrated. [2].



**Fig.1** (a) Attenuated and corrected THz waveforms using 10 Si wafers as attenuators vs. the original strong THz signal. (b) THz spectrum of the corrected THz signal with 10 Si wafers vs. that of the original one.

**References**

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**XiaoYu Peng** is Professor of Research Centre for Terahertz Technology, Chongqing Institute of Green and Intelligent Technology (CIGIT), Chinese Academy of Sciences (CAS). He received his PhD in optics from the Institute of Physics of CAS in 2005. From January 2006 to the end of October 2008, he worked as a postdoctor and a guest scientist in the Institute for laser and Plasma Physics, Heinrich Heine University Duesseldorf, Germany. In December 2008, he joined the Institute of Materials Research and Engineering, Agency for Science, Technology and Research (**A\*STAR**) of Singapore as a research scientist. In 2014, He joined CIGIT as a professor.



His current research interests include: broadband terahertz wave generation, detection, and applications; powerful, high-field terahertz source based on laser-pumping and its applications; terahertz modulators, sensors or detectors based on micro/nano structures.

For more information, please visit <http://peopleucas.ac.cn/~0041117?language=en>.

**Session A9**

**A42**

**9:15 - 9:40 AM Room A June 22**

## The fascinating split-ring-resonators: progress in design, fabrication and applications of terahertz metamaterials

MEI ZHU

School of Physics & Electronic Engineering, Taishan University

525 Dongyue Road, Tai'an City, Shandong Province, China

Email: zm\_1805@163.com

### Abstract

Metamaterials with many unique optical properties are made of periodically arranged sub-wavelength metallic structures that are able to couple to external electromagnetic (EM) waves. One of such structures is the commonly used split-ring-resonators (SRR). In this talk, I will discuss and demonstrate some new progress we made on SRR-based terahertz metamaterials. By looking into the coupling between SRRs and the effect of incident polarization, we proposed a way to continuously modulate their resonances, changing the transmission intensity at resonant frequency from 20% to 80%.[1] We also designed a SRR-based polarization-insensitive broadband filter in THz range and discovered its effect in eliminating asymmetric characteristics in device structure. [2] A stop band with bandwidth of as large as 1.40 THz was achieved. To improve the fabrication process, a facile metal transfer method was employed to create SRR patterns on PDMS surface, planar and otherwise, as well as PDMS-coated surfaces, such as paper, fabric and leaf. [3] Lastly, a design of 3D THz metamaterial device was proposed to be used in biomedical field for cancer cell studies, exploiting its structural similarities with the single-cell-capturing microfluidic devices.

### Acknowledgements

Financial support from the National Natural Science Foundation of China (No. 61605139), the Natural Science Foundation of Shandong Province (No. ZR2016FQ15) and the Science and Technology Planning Project of Higher Education of Shandong Province (No. J16LJ10) is acknowledged.

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**Mei Zhu** got her Bachelor's degree and Ph.D. degree from National University of Singapore (NUS) in 2009 and 2013, respectively. Her Ph.D. work focused on creation and applications of polymer-based micro- and nanostructures. After graduation, she worked in NUS as a research fellow for another year, during which she worked on the theory, design and fabrication of terahertz (THz) metamaterials. She returned to China in 2015, and has since then been a lecturer in School of Physics & Electronic Engineering, Taishan University.



Her current research interests include THz metamaterials for biomedical applications, and novel THz metamaterial designs and fabrication processes.

**Session A9**

**A43**

**9:40 - 10:05 AM Room A June 22**

## Broadband terahertz absorber based on sinusoidally-patterned graphene

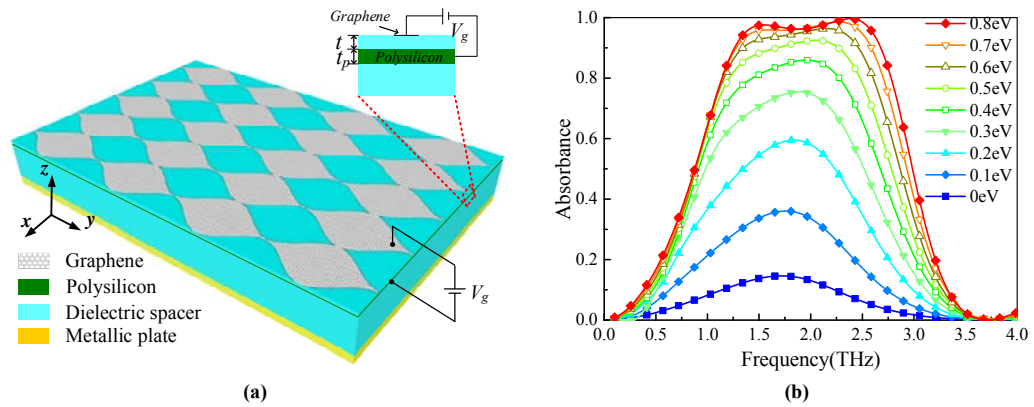
LONGFANG YE\*, YAO CHEN

Institute of Electromagnetics and Acoustics, and Department of Electronic Science, Xiamen University,  
Xiamen 361005, China

Email: lfye@xmu.edu.cn

### Abstract

Broadband terahertz absorbers have recently attracted considerable attention for their promising applications in terahertz trapping, sensing, imaging, and detecting. In this work, an efficient approach to achieve broadband terahertz absorber based on sinusoidally-patterned graphene with nearly 100% absorption is demonstrated [1]. As shown in Fig. 1(a), the proposed absorber is composed of a net-shaped periodically sinusoidally-patterned graphene sheet on the top, a thin gating layer embedded dielectric spacer in the middle, and a metallic reflecting plate on the bottom. We assume the material of the dielectric spacer, the gating layer and metallic plate are the polyethylene cyclic olefin copolymer (Topas) with the permittivity of  $\epsilon_{rt} = 2.35$  [2], and the polysilicon with the permittivity of  $\epsilon_{rp} = 3$  [3], and gold, respectively. The surface conductivity of the single-layered graphene is obtained from the Kubo formula [4]. The polysilicon gating layer is placed beneath the graphene sheet to control the graphene conductivity via electrostatic doping of the graphene by applying a DC voltage  $V_g$ . By introducing such a unique gradient width modulation of the unit graphene sheet structure, the continuous plasmon resonances of the absorber can be excited, and over 65% normalized bandwidth of 90% terahertz absorbance can be achieved under normal incidence for both TE and TM polarizations. As one of the most exciting characteristics, the broadband absorption of this absorber are insensitive to the incident angles and the polarizations. The absorbance remains more than 70% even the incident angles reach  $60^\circ$  for both polarizations. Furthermore, compared to conventional multi-resonator or multi-layered structures, the continuous net-shaped single-layered graphene structure can greatly simplify the electrostatic gating structure in achieving flexible tunability. By controlling the chemical potential of the graphene, the peak absorbance can be continuously tuned from 14% to 100%, as shown in Fig. 1(b). This work offers a new perspective on the design of graphene-based tunable terahertz broadband absorbers. The design scheme can be easily scaled to the infrared or visible regimes.

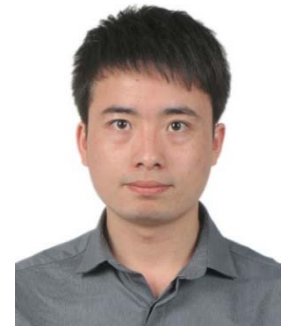


**Fig. 1** (a) Schematic of the proposed graphene-based broadband terahertz absorber, where the net-shaped periodically sinusoidally-patterned graphene sheet is placed on a dielectric spacer supported on a metallic reflecting plate, where a thin polysilicon layer is placed beneath the graphene sheet as a gating layer to control the graphene conductivity via a DC voltage  $V_g$ . (b) Normal-incidence absorbance in the TE polarization of the graphene-based absorber for various values of the graphene chemical potential  $\mu_c$ , where the peak absorbance increases from 14% to nearly 100% when  $\mu_c$  is tuned from 0 to 0.8 eV.

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**Longfang Ye** received the Ph.D. degree in electromagnetic field and microwave technology from the University of Electronic Science and Technology of China in June 2013. He was with Massachusetts Institute of Technology as a visiting Student from October 2011 to January 2013. Since July 2013, he has been with Xiamen University, where he is currently an Assistant Professor of Electronic Science.



His research interests include microwave circuits and antennas, terahertz waveguides, metamaterials, photonics, and graphene-based devices.

For more information, please visit <http://ema.xmu.edu.cn/index.php?c=product&id=35>;  
<http://cpst.xmu.edu.cn/pmee/user/75>



**Session A10**

**A44**

**10:20 - 10:45 AM Room A June 22**

## Engineering rainbow trapping and releasing in ultrathin THz plasmonic graded metallic grating strip with thermo-optic material

GENQUAN HAN

Wide Bandgap Semiconductor Technology Disciplines State Key Laboratory, School of Microelectronics, Xidian University, Xi'an 710071, China

Email: hangenquan@gmail.com

### **Abstract**

In this paper, we propose an ultrathin THz plasmonic metallic strip based on graded grating structure with thermo-optic material, which exhibits a strong engineering of trapping and releasing electromagnetic waves in terahertz regimes. The dispersion properties of the ultrathin spoof slow-wave plasmonic graded grating waveguide are characterized using the finite element method, and the propagation characteristics of the grating structures are thoroughly analyzed by the dispersion curves, electric field magnitude distribution, and electric field vertical distribution. The gradient grating waveguide is demonstrated to be an ideal slow-wave system for trapping and releasing surface plasmon polaritons (SPPs) waves through tuning the refractive index of the thermo-optic material. The reflected location for the SPPs waves on the graded corrugated metal strip at 1.1 THz at different temperatures are compared. It is proved that such ultrathin gradient grating waveguide provides an excellent performance for trapping and releasing surface waves at THz, which permits applications for future optical communications.

**Genquan Han** received his B.S. degree in Department of Materials Science and Engineering from Tsinghua University, Beijing, China, in 2003, and Ph.D. degree in Institute of Semiconductors, Chinese Academy of Sciences in 2008. From 2008 to 2013, he was a Research Fellow at the National University of Singapore. From 2013 to 2015, he was a professor in Chongqing University, China. In 2015, he joined Xidian University, China, as a professor.



His current research interests include advanced CMOS, photonics devices, and wide bandgap materials and devices.

*Session A10*

*A45*

*10:45 - 11:10 AM Room A June 22*

## Micro-fabricated L-shape metasurface terahertz biosensor

JUN ZHOU

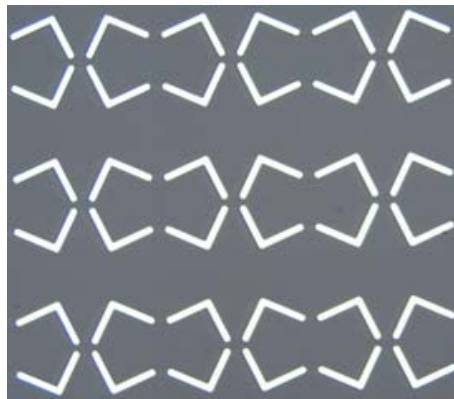
University of Electronic Science and Technology of China

No. 4, Section 2, North Jianshe Road, Chengdu, China

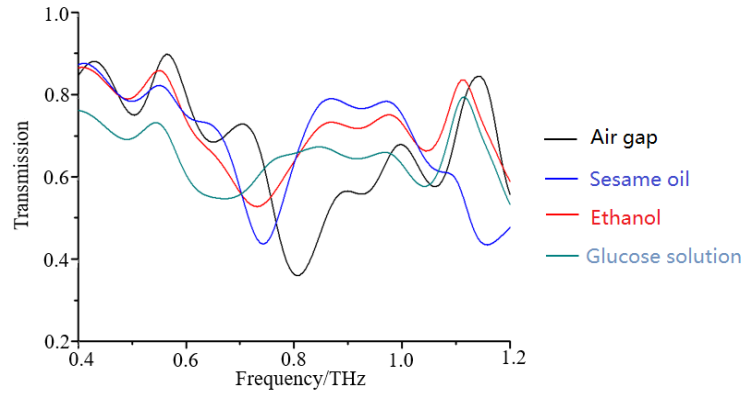
Email: zhoujun123@uestc.edu.cn

### **Abstract**

In recent years, more and more attention has been paid on the research and development of terahertz (THz) technologies all over the world. Biosensing is one of the most important applications of THz waves. Metasurface is an artificial two-dimensional material with flexible structures and good electromagnetic wave control capability, which is very suitable for THz wave control and sensing. In this work, a L-shape metasurface THz biosensor was designed, simulated, optimized, micro-fabricated, and finally tested by the time-domain spectroscopy (TDS) system. The simulation and experimental results agree with each other very well. The conclusions show great advantage of metasurface for the THz biosensing application, especially when it is combined with the microfluidic technology in the near future.



*Fig.1 Structure of sensing array*



**Fig.2** Measured results of some liquid samples

### References

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**Jun Zhou** is Associate Professor of Physical Electronics. He is a Member of IEEE and OSA. He is now working in the Terahertz Research Center, University of Electronic Science and Technology of China. He has authored/coauthored more than 50 technical journals and conference papers.

His current research interests include computational electromagnetics, terahertz transmission, spectroscopy and imaging.



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<http://en.uestc.edu.cn/index.php?m=content&c=index&a=show&catid=79&id=4959>  
or <http://222.197.183.99/TutorDetails.aspx?id=1411>.

Session A10

A46

11:10 - 11:35 AM Room A June 22

## Intensity and spectral changes in terahertz quantum cascade lasers induced by the injection of near-infrared optical pulses

Y. SAKASEGAWA, N. SEKINE, S. SAITO, A. KASAMATSU, AND I. HOSAKO

National Institute of Information and Communications Technology

4-2-1 Nukui-Kitamachi, Koganei, Tokyo 184-8795, Japan

Email: ysaka@nict.go.jp

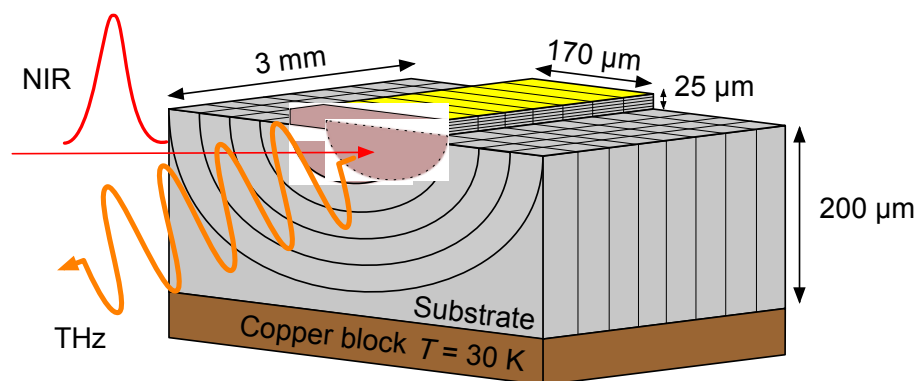
M. ASHIDA

Graduate School of Engineering Science, Osaka University

Toyonaka 560-8531 Osaka, Japan

### Abstract

Terahertz quantum cascade lasers (THz-QCLs) have attracted much attention as possible carrier sources for ultra high-speed wireless communications in the future, which owes to their high output powers and the absence of relaxation oscillations in QCLs. We have recently reported a photogenerated carrier-based optical-to-THz modulation scheme for THz-QCLs [1]. In the presentation, the intensity and spectral changes in THz-QCLs induced by photo-injected carriers at low temperature will be discussed together with the relevant relaxation mechanisms for the injected carriers. Furthermore, to obtain a quantitative understanding of the rich phenomena by the optical injection, we developed a global simulation scheme applicable to a wide variety of optical excitation experiments on QCLs including strong excitation densities (Fig. 1) [2]. With the most of internal parameters, e.g., electron temperatures, scattering times, gains, and waveguide loss, treated as spatiotemporal and carrier density-dependent, the rate equation was solved to obtain the number of photon in the cavity. The output power (converted from the number of photons using the time-varying reflectivity at the cavity facet) well reproduces the experimental results.



**Fig.1** Model grid for the analysis of the optically excited QCL

### **Acknowledgement**

N.S. acknowledges funding by Collaborative Research Based on Industrial Demand of the Japan Science and Technology Agency.

### **References**

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**Session A10**

**A47**

**11:35 - 12:00 PM Room A June 22**

## THz surface Emission spectroscopy and applications

YUAN YUAN HUANG, LIPENG ZHU, XINLONG XU \*

Shaanxi Joint Laboratory of Graphene,

State Key Laboratory for Incubation Base of Photoelectric Technology and Functional Materials, and Institute of Photonics & Photon-Technology,

Northwest University, Xi' an, China

\*Email: xlxuphy@nwu.edu.cn

### Abstract

Terahertz (THz) wave, bridging electronics and photonics in the electromagnetic spectrum, features many exotic properties and promising applications. However, because of low THz emission efficiency, less sensitive detectors, and few manipulating devices, THz wave is still on the horizon for practical applications since 1980s. With the application of femtosecond laser, THz surface emission spectroscopy has also been developed to serve as a sensitive and contactless tool for the optoelectronic measurement of semiconductor surfaces and interfaces. When a femtosecond laser beam impinges on the semiconductor surface, photocarriers or photodipoles are excited, which then induce THz radiation with the mechanism of photoconductivity or optical rectification. As the THz surface emission is sensitive to the surfaces and interfaces, the modification of the semiconductor surface provides a significant strategy for the design and performance evaluation of many electronic and optoelectronic devices for THz applications. In this talk, we will discuss the THz radiation mechanism for traditional semiconductors by changing the crystal orientation, exciting laser intensity, surface condition, and so on [1-4]. We will also discuss THz radiation from two-dimensional layered semiconductors under linearly polarized femtosecond laser excitation.

### References

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**Xinlong Xu** is Professor of Physics in Institute of Photonics & Photon-Technology, Northwest University, China. He is a deputy director of Shaanxi Joint Lab of Graphene (Northwest University). He is a Member of Shaanxi Province Physical Society. He was the recipient of the New-star in Science and Technology in Shaanxi Province for his contributions to the field of nano and THz science and technology in 2012.



His current research interests include nanooptics, THz photonics, and metamaterials.

For more information, please visit <http://physics.nwu.edu.cn/index.php?s=/Public/teacher/id/91>.

**Session A11**

**A48**

**14:00 - 14:25 PM Room A June 22**

## Design and electrochemical performance of nano-micro structured porous materials

YINGKE ZHOU

The State Key Laboratory of Refractories and Metallurgy  
College of Materials and Metallurgy, Wuhan University of Science and Technology  
Wuhan 430081, P. R. China  
Email: zhouyk888@hotmail.com

### **Abstract**

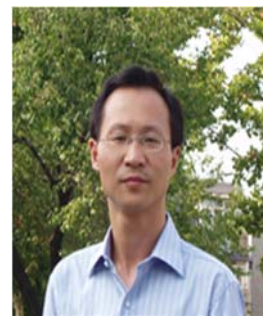
Graphene and carbon nanotube present unique structure and excellent properties, such as high specific surface area, high conductivity, high thermal conductivity, etc., and play an increasingly important role in the electrochemical energy storage and conversion. The doping of nano-carbon with nitrogen and boron can modulate the electron and energy band structure, and further improve its physical and chemical properties. The pore structure, pore size distribution and wall thickness of the electroactive material display important effect on the electrolyte infiltration, the ion transport and adsorption, and the overall performance of the battery. The use of doped nano-carbon and porous composite structure can improve the conductivity and the electrochemical surface area and reaction sites of the electroactive materials, and significantly increase the efficiency of energy storage and conversion.

This presentation focuses on some progresses of the doped nano-carbon and porous composite structures, including the following three aspects: (1) The controllable synthesis and electrochemical lithium insertion characteristics of the porous electrode materials. Porous materials have been widely used in a variety of fields, but their large-scale controllable synthesis is still a considerable challenge. We have designed a novel templated freeze-drying method to conveniently control the porous properties of materials, which has been successfully applied to the synthesis of various porous phosphates, oxides and composites, and the electrochemical lithium storage properties have been explored. (2) The porous lithium iron phosphate and nitrogen-doped graphene composite. Three-dimensional porous microspheres composed of LiFePO<sub>4</sub> and nitrogen-doped graphene have been synthesized by a solvothermal method. The effect of graphene doping on the nucleation and growth of LiFePO<sub>4</sub> and the influence of the unique self-assembled porous microsphere structure on the electrochemical lithium insertion performance have been studied. (3) Supercapacitance properties of doped graphene. A series of dopant graphene materials have been facilely synthesized by a thermal solid state reaction. The regulation of doping configuration on the electronic structure of graphene and the influence on the supercapacitance have been systematically studied. The relevant mechanisms have been proposed and some phenomena in the literature have been reasonably explained.

This work was supported by the National Natural Science Foundation of China (No. 51372178) and the Natural Science Foundation for Distinguished Young Scholars of Hubei Province of China (No. 2013CFA021).

**Keywords:** energy storage and conversion; doped nano-carbon; porous structure

**Yingke Zhou** is a Professor of Materials Chemistry and Director of the Lab of New Energy Materials of Wuhan University of Science and Technology, and he is a Chutian scholar of Hubei Province. He has published more than 60 papers in peer reviewed journals, which have been cited for more than 3000 times, and received several patents. His research has been supported by the National Natural Science Foundation of China, the Science and Technology Department of Hubei Province, and the industry projects. He has received three Ministerial and Provincial Science and Technology Awards, and has been invited to review papers for more than 30 international journals, such as *Energy & Environmental Science*, *Carbon*, *Journal of Power Sources*, *Chemical Communications*, etc.



His current research interests include new energy materials, lithium-ion batteries, fuel cells and supercapacitors.

**Session A11**

**A49**

**14:25 - 14:50 PM Room A June 22**

## Molecular Insights into Electrical Double Layers in Graphene-Based Supercapacitors

SHENG BI, GUANG FENG, SONG LI

State Key Laboratory of Coal Combustion

Huazhong University of Science and Technology, Wuhan, Hubei 430074 China

Email: chrishengbee@hust.edu.cn, gfeng@hust.edu.cn

NINA BALKE

Center for Nanophase Materials Sciences

Oak Ridge National Laboratory, Oak Ridge , TN 37831, USA

Email: balken@ornl.gov

PETER T. CUMMINGS

Department of Chemical and Biomolecular Engineering

Vanderbilt University, Nashville, TN 37235, USA

Email: peter.cummings@vanderbilt.edu

RUI QIAO

Department of Mechanical Engineering

Virginia Tech, Blacksburg, Virginia 24061, USA

Email: ruiqiao@vt.edu

ALEXEI A. KORNYSHEV

Department of Chemistry

Imperial College London, SW7 2AZ London, UK

Email: a.kornyshev@imperial.ac.uk

### **Abstract**

Recently nano-structural carbons have become the most widely used electrode materials in supercapacitor community, because of their high specific surface area, good electrical conductivity, chemical stability in a variety of electrolytes, and relatively low cost. In particular, graphene-based carbons are emerging as an auspicious candidate due to the unique feature of graphene. Among electrolytes used for supercapacitors, ionic liquids (ILs) have been becoming a promising class of them, owing to their exceptionally wide electrochemical stability window, excellent thermal stability, non-volatility and relatively inert nature. Despite considerable work on supercapacitor with graphene-based carbon as electrodes, the details of what happens under nano-confinement, including pores, still require in-depth exploration especially for IL electrolytes.

We studied the interfacial phenomena occurring between ILs and graphene-based electrodes in supercapacitors, using the combined molecular dynamics (MD) simulation by modeling ILs-based EDLs at planar, cylindrical, spherical electrode surfaces and inside electrode pores at nano/micro-scale. This talk would include:

- 1) MD modeling on ILs-based EDLs at open surfaces (e.g., planar, cylindrical, spherical, with defects, etc.)<sup>[1-2]</sup> and the integration with experiments (e.g., atomic force microscopy, AFM),<sup>[3-4]</sup> which would focus on the EDL structure and its influence from ion size, ion type, applied potential, electrode curvature, etc.
- 2) MD modeling on ILs-based porous carbon supercapacitors<sup>[5-7]</sup>, which would embody the pore size effects on capacitance, the ion dynamics under porous confinement, and pore expansion during charging.
- 3) The anatomy of electrosorption for water in ionic liquids at electrified interfaces,<sup>[8]</sup> which would show, for the first time, the work on the adsorption of water on electrode surfaces in contact with humid ILs.

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**Guang Feng** is a professor in State Key Laboratory of Coal Combustion and School of Energy and Power Engineering in Huazhong University of Science and Technology (HUST), China. He is a Member of Sigma Xi, AIChE, APS, ACS, ECS, and RSC. He was awarded by Hubei Provincial 100-Talents Program in 2013. He has published 3 book chapters (by Wiley-VCH, Springer and CRC/Taylor & Francis, respectively) and 45 papers (6 invited articles) in peer-reviewed journals including *Nano Letters*, *Advanced Energy Materials*, *ACS Nano*, *Nano Energy*, etc.



His current research is mainly focused on study of micro-/nano-scale interface and transport phenomena in applications of energy storage, capacitive deionization for desalination and water treatment, and carbon capture and utilization.

For more information, please visit <http://itp.energy.hust.edu.cn>.

**Session A11**

**A50**

**14:50 - 15:15 PM Room A June 22**

## Preparation of novel microporous organic frameworks

TENG BEN

Department of Chemistry, Jilin University,

Changchun, 130012, China

Email: tben@jlu.edu.cn

### Abstract

Porous materials have attracted much attention all over the world, because of their wide range of applications in the areas of catalysis, gas separation and gas storage.[1] Porous organic frameworks (POFs) can find potential applications owing to high Brunauer-Emmett-Teller (BET) surface area (PAF-1[2] exhibits BET surface areas as high as  $5640 \text{ m}^2 \text{ g}^{-1}$ ), exceptional physicochemical stability and low skeleton density. However, for the intrinsic low conductivity of mostly POFs, it still remains a challenge to apply POFs as supercapacitor. Hence charged POFs or direct carbonized POFs may be good solution to improve the conductivity of POFs. Moreover, to the best of our knowledge, most of POFs are uncharged and only few reports on charged porous organic frameworks. Herein, we describe the synthesis of a series of novel charged POFs using potassium tetrakis(4-bromopyrazolyl) borate and tetrakis(4-chlorophenyl) phosphonium bromide as monomers in different ratios by a Nickel(0)-catalyzed Yamamoto-type Ullmann coupling reaction followed by carbonization of the charged POFs to obtain a series of carbonized PAFs. The carbonized PAFs thus obtained were found to exhibit high capacitances.

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**Teng Ben** received his Ph.D. in 2002 from Jilin University in polymer science. After graduation, he joined the faculty at Jilin University, working with Prof. Zhongwen Wu as a lecturer. In 2005, he moved to Prof. Eiji Yashima's group at the Nagoya University in Japan as a postdoctoral researcher. In 2008, he moved back to Jilin University as an Associate Professor and was promoted to a Professor in 2010. His research interests include the fundamental understanding of host-guest interactions in nanoporous materials, gas storage and separation using porous organic frameworks.





## Session A11

A51

15:15 - 15:40 PM Room A June 22

## Porous Carbons and Polymers for Gas Mixture Separation

YUNFENG ZHAO\*

Tianjin Key Laboratory of Advanced Functional Porous Materials, Institute for New-Energy Materials and Low-Carbon Technologies, Tianjin University of Technology, Tianjin, 300384

Email: yfzhao@tjut.edu.cn

**Abstract**

The greenhouse gas effect that causes global warming is largely associated with the CO<sub>2</sub> emissions from the burning of fossil fuels in power plants and combustion engines. It is therefore critical to develop effective methods for CO<sub>2</sub> capture and sequestration (CCS) from post-combustion effluents, such as power plant flue gases that typically comprise 3-15% CO<sub>2</sub> and more than 70% nitrogen (N<sub>2</sub>) under a pressure of 1 bar.

We developed various effective strategies (N-doping, surface functionalization, extra-framework ions, molecular design, and pore size engineering) for enhancing the CO<sub>2</sub> adsorption capacity and selectivity of carbonaceous adsorbents.<sup>[1-4]</sup>

In addition, porous organic polymer (POPs) has attracted more and more attentions because of low-cost, designable and easy-modification. POPs have displayed promising potential in the field of gas adsorption and separation. We have prepared a series of POPs for CO<sub>2</sub> and CH<sub>4</sub> capture and related mix gas separation.

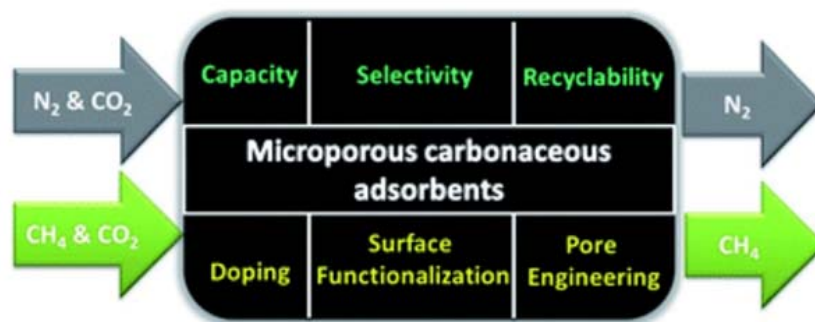


Fig. 1

**Reference**

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**Yunfeng Zhao** received his Bachelor (2004) and PhD (2009) degree from Jilin University, China. He worked in King Abdullah University of Science and Technology (KAUST) in the Kingdom of Saudi Arabia, as a Post-Doc from 2009 to 2015. He joined Tianjin University of Technology in China in 2015 as a professor. He received “Thousand Youth Talents Plan Project of Tianjin City” and “131 Innovative Talents Training Project of Tianjin City (1st Level)” in 2016. His research is mainly focused on nanoporous materials and their applications in adsorption, separation, and catalysis. He has published more than 40 peer-reviewed journal articles with the citation over 1100 times.



**Session A12**

**A52**

**16:00 - 16:25 PM Room A June 22**

## **Controllable Synthesis of N-Doped and Dually Doped Mesoporous Carbons for Adsorption and Catalysis Applications**

ZHANGXIONG WU, ZHI CHEN, XINGMIN GAO, ZHUJUN ZHANG

School of Chemical and Environmental Engineering, College of Chemistry, Chemical Engineering and Materials Science, Soochow University

NO. 199, Ren-Ai Road, Suzhou Industrial Park, Suzhou, Jiangsu 215123, China

Email: zhangwu@suda.edu.cn

### **Abstract**

Mesoporous carbon materials are being in vogue because of their intriguing properties and wide potentials. Doping of heteroatoms, especially N, in carbons have attracted enormous interests owing to its capability in enhancing or expanding their applicability in separation, energy conversion and catalysis. In addition, N-doping can further boost dually doped carbons, such as with S and metal as the second dopant. Such a dual doping could possibly optimize material property and maximize performance through synergistic effects. In this talk, several synthetic methods, such as post modification [1-2], one-step solvent-free nano-confining synthesis [2-3] and spray-drying-assisted assembly [5], for the synthesis of heteroatom (singly or dually) porous carbon materials with different porosities and structures will be introduced and discussed. Furthermore, the controllable synthesis of metal/heteroatom dually doped mesoporous carbons with desirable fascinating properties will be introduced. The demonstrations of these materials in typical adsorption, such as arsenic removal and CO<sub>2</sub> capture, and typical catalysis, such as oxygen reduction, biodiesel production and dehydrogenation/hydrogenation coupling reactions, will be presented and their structure-performance correlations will be discussed.

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**Zhangxiong Wu** is Professor of Chemical Engineering and Associate Director of Particle Technology Engineering Laboratory (under the China Petroleum and Chemical Industry Association) at Soochow University. He was selected by the Thousand Youth Talents Plan of China in 2015. He was the recipient of “Young Investigator Award” (awarded in the 6<sup>th</sup> Asian Particle Technology Symposium) for his contributions to the field of porous particles in 2015.



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<http://www.scee-suda.com/index.aspx?lanmuid=75&sublanmuid=640&id=16>

Session A12

A53

16:25 - 16:50 PM Room A June 22

## Accelerating the extracellular electron transfer of *Shewanella oneidensis* MR-1 by decorating cytochromes with carbon quantum dots and MWNTs

PENG ZHANG, JIA LIU, YUJIE FENG\*

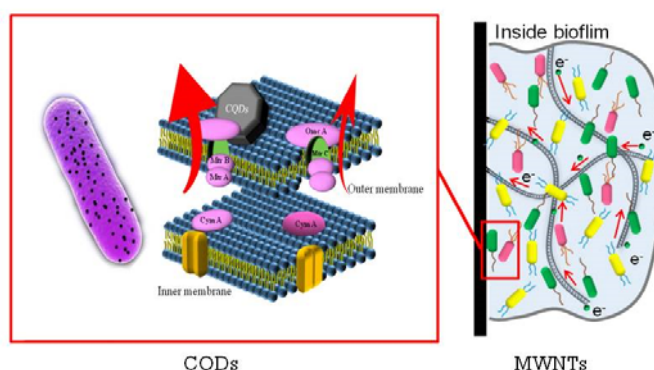
Harbin Institute of Technology

No 73 Huanghe Road, Nangang District, Harbin 150090, Heilongjiang, China

Email: yujief@hit.edu.cn

### Abstract

Microbial extracellular electron transfer process plays important roles in the areas of energy production, environmental remediation and geochemical cycle systems [1]. However, the low electron transfer efficiency restricts its further application. In our research, the current generation is improved by modifying of *Shewanella oneidensis* MR-1 with carbon quantum dots (CQDs). The proper addition of CQDs increases the current by more than 5 times, by means of enhancing the anode biofilm formation and flavins extraction. Further mechanism analyse showed that CQDs could combine with cytochrome c on the outer membrane and intercalate in the electron transfer pathway for faster electron transfer rate. In another study, a bacteria/MWCNT hybrid biofilm is fabricated by effective MWCNT insertion in the anode biofilm with an adsorption-filtration method. The current density, power density and coulombic efficiency are increased by 46.2%, 58.8% and 84.6%, respectively, while the start-up time is reduced by 53.8%, compared with natural grown biofilm.



**Fig.1** The diagram of enhanced microbial extracellular electron transfer with CQDs and MWNTs

### References

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**Yujie Feng** is a Professor of Harbin Institute of Technology. She is currently the Deputy Director of the State Key Laboratory of Urban Water Resource and Environment (HIT) in China. She is also Visiting Professor in Penn State University, USA and IWA Fellows. She focused on the research on wastewater treatment and energy/resources recovery, especially on the toxic industrial wastewater treatment, energy recovery, risk evaluation and recycling. She pioneered the development of microbial electrochemical system, coupled with functional nano-materials in wastewater treatment and ecological remediation of polluted urban water system.



## Session A12

A54

16:50 - 17:15 PM Room A June 22

## Application of transition-metal dichalcogenides beyond general electronics

YIJIN ZHANG

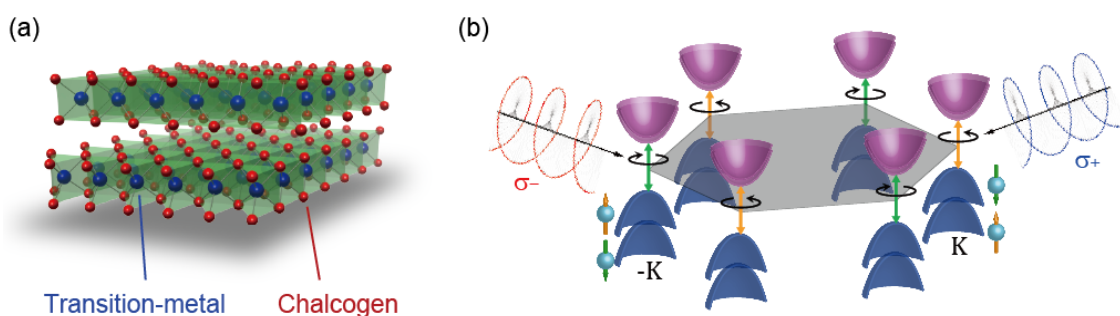
Max Planck Institute for Solid State Research

Heisenbergstr. 1, 70569 Stuttgart, Germany

Email: Y.Zhang@fkf.mpg.de

**Abstract**

Transition-metal dichalcogenides (TMDs) are novel layered materials for various kind of application. In particular, those formed in hexagonal prismatic structure (Fig. 1a) with group-VIB transition-metal are semiconductors in nature and show good transistor performance and strong light-matter interaction. However, the potential application of group-VIB TMDs is not only limited to such general electronics and optics, but also covers next-generation electronics of spintronics and valleytronics including the coupling to the optical polarization (Fig 1b) [1]. Owing to the lack of the inversion centre in the individual layer, the six conduction band minima and valence band maxima at the edge of the hexagonal Brillouin zone split into two groups, creating a valley degree of freedom. Optical interband transition at these high symmetry points are further coupled to the helicity of light. In addition, the heavy transition-metal elements leads to a large spin-orbit interaction and a consequent spin splitting. Here, I will report our recent research aiming at next-generation electronics, including optoelectronic device utilizing valley degree of freedom [2,3] and the fundamental investigation of the spin relaxation in TMDs [4].



**Fig.1** Crystal structure (a) and band structure (b) of group-VIB transition-metal dichalcogenides.



## **References**

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**Session B9**

**B36**

**8:00 - 8:25 AM Room B June 22**

## Nano Photocatalytic Materials Design Toward Small Molecular Hydrocarbons Oxidation

ZHIGUO YI

Fujian Institute of Research on the Structure of Matter,  
Chinese Academy of Sciences, Fuzhou 350002  
Email: zhiguo@fjirsm.ac.cn

### **Abstract**

The search for active catalysts that efficiently oxidize methane under ambient conditions remains a challenging task for both C1 utilization and atmospheric cleansing [1-6] Here, we show that when the particle size of zinc oxide is reduced down to the nanoscale, it exhibits high activity for methane oxidation under simulated sunlight illumination, and nano silver decoration further enhances the photo-activity via the surface plasmon resonance. The high quantum yield of 8% at wavelengths <400 nm and over 0.1% at wavelengths ~470 nm achieved on the silver decorated zinc oxide nanostructures shows great promise for atmospheric methane oxidation. Moreover, the nano-particulate composites can efficiently photo-oxidize other small molecular hydrocarbons such as ethane, propane and ethylene, and in particular, can dehydrogenize methane to generate ethane, ethylene and so on. On the basis of the experimental results, a two-step photocatalytic reaction process is suggested to account for the methane photo-oxidation.

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**Zhiguo Yi** is a Professor of Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences.

His current research interests include photocatalytic chemistry, Ferroelectric physics and solid state ionics.

For more information, please visit

<http://www.fjirsm.cas.cn/research/R2/yzg/yzgktzz/>



**Session B9**

**B37**

**8:25 - 8:50 AM Room B June 22**

## Ternary Nanostructured Photocatalysts for Photoelectrochemical Water Splitting

MENG NAN CHONG<sup>1,2\*</sup>, YI WEN PHUAN<sup>1</sup>

<sup>1</sup>School of Engineering, Chemical Engineering Discipline, Monash University Malaysia, Jalan Lagoon Selatan, Bandar Sunway, Selangor Darul Ehsan 47500 Malaysia

<sup>2</sup>Sustainable Water Alliance, Monash University Malaysia, Jalan Lagoon Selatan, Bandar Sunway, Selangor Darul Ehsan 47500 Malaysia

\*Corresponding author: Associate Professor Dr. Meng Nan Chong

School of Engineering, Chemical Engineering Discipline, Monash University Malaysia, Jalan Lagoon Selatan, Bandar Sunway, Selangor Darul Ehsan 47500 Malaysia

Ph: +60 3 5514 5680; Fax: +60 3 5514 6207;

Email: Chong.Meng.Nan@monash.edu

### Abstract

The world's population is growing continuously and in close proportionality to the demand on fossil fuels, which may lead to its depletion in the coming decades. The ability to harness energy from renewable resources is highly desirable for a sustainable energy economy. In recent years, photoelectrochemical (PEC) water splitting processes based on Earth-abundant semiconductor photocatalysts have gained considerable research interests for resolving energy and environmental issues. The PEC water splitting that mimics the natural photosynthesis process can convert solar energy into a storable form of hydrogen (H<sub>2</sub>) energy, which is a good energy vector to meet the escalating energy demand. To date, however, almost all singular semiconductor photocatalysts used demonstrated poor PEC performance for solar-to-H<sub>2</sub> energy conversion. In this study, two different novel ternary nanostructured hematite-based photocatalysts of eRGO/C60/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and eRGO/NiO/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> were synthesized, characterised and tested as photoanodes toward PEC water splitting application. The ternary nanostructured hematite-based photoanodes were characterised using FE-SEM, EDX, XRD, XPS, as well as Raman, UV-Vis and EIS spectroscopic methods. It was found that the ternary nanostructured photoanodes of eRGO/C60/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and eRGO/NiO/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> showed 5-fold and 9-fold enhancement in current density and significant reduction in charge transfer resistance when compared to the pristine hematite photoanode. In this instance, the enhancement in PEC performance of ternary nanostructured eRGO/C60/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> photoanode was attributed to the electron scavenging property of C60 as well as the highly conducting eRGO property that have mitigated the high interfacial recombination rate of photogenerated electron-hole pairs. Whilst for the ternary nanostructured eRGO/NiO/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> photoanode, eRGO transferred the electrons efficiently in the *p-n* heterojunction without causing substantial bulk recombination. Additionally, the internal electrostatic field in eRGO/NiO/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> could facilitate the effective separation of photogenerated electron-hole pairs so that more holes could participate in the water oxidation reaction instead of recombination process. It is anticipated that the fundamental understanding gained through

this study is helpful to design and construct high-performance photoelectrodes for the application in PEC water splitting in the near future.

**Session B9**

**B38**

**8:50 - 9:15 AM Room B June 22**

## Photocatalytic Degradation of Polybrominated Diphenyl Ethers on TiO<sub>2</sub>-based composites

NAN WANG, LIHUA ZHU

School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, 430074, Wuhan, China  
Email: nwang@hust.edu.cn, lh Zhu63@hust.edu.cn

MING LEI, HEQING TANG

College of Resources and Environmental Science, South-Central University for Nationalities, 430074, Wuhan, China.  
Email: tangheqing@mail.scuec.edu.cn

### **Abstract**

Polybrominated diphenyl ethers (PBDEs) are widely used as flame retardants, and become a new class of global contaminants. Because PBDEs possess typical characteristics of persistent organic pollutants (POPs) like persistent, bioaccumulation, and biotoxicity, their elimination therefore attracts much attention of researchers.

The reductive debromination is a common strategy to treat PBDEs. Among various reductive methods, the photogenerated electron of TiO<sub>2</sub> is considered to be highly efficient to reduce decabromodiphenyl ether (BDE209) [1]. However, this leads to accumulation of brominated intermediates, but the debromination products with less bromine atoms are much more difficult to get further reductive debromination.

To promote the photocatalytic reductive debromination, we developed several TiO<sub>2</sub>-based composites including reduced graphene oxide (RGO) loaded TiO<sub>2</sub> (RGO/TiO<sub>2</sub>), Ag/TiO<sub>2</sub>, and CuO/TiO<sub>2</sub> to reduce BDE209 and/or 2,2',4,4'-tetrabromodiphenyl ether (BDE47) [2-4]. These heterostructured photocatalysts have two beneficial roles: charge separation in space, and enhanced adsorption of PBDEs. Thus, the photocatalytic reduction of PBDEs was greatly improved. However, the complete debromination of PBDEs to diphenyl ether through the photocatalytic reduction process is rather difficult. For example, although all the added BDE47 was rapidly reduced, the debromination efficiency was still less than 50% over Ag/TiO<sub>2</sub> and CuO/TiO<sub>2</sub> [3, 4]. This is because that the reduction of low-brominated PBDEs is rather difficult, due to their weak electron affinity.

Although most studies indicate that BDE209 is strongly resistant to oxidation, we firstly demonstrated that the h<sup>+</sup>/•OH-involved oxidative degradation of BDE209 took place slowly in the UV-irradiated TiO<sub>2</sub> aqueous dispersions [5]. We also noted that the oxidation of BDE209 is much slower than the following oxidation of the less-brominated organic intermediates. Since the highly brominated PBDEs are more easily reduced, and the lower brominated PBDEs become more susceptible to the oxidation, we then developed an effective “one-pot” photocatalytic system for driving concurrently the pre-reduction and consecutive oxidation of BDE47.

## **References**

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**Heqing Tang** is Professor of Chemistry and Director of College of Resources and Environmental Science, South-Central University for Nationalities (Wuhan, China).



His current research interests include the removal of toxic organic pollutants by the advanced oxidation technologies like photocatalysis, Fenton and Fenton like catalysis. He has developed some approaches to improve the (photo)catalytic behavior of metal oxides nanoparticles through various surface modifications such as by depositing metallic hydroxide, in situ adsorbing ligands, the formation of charger-transfer complex, and the construct of heterosturctured catalysts. These researches have been supported by the National Natural Science Foundation. He has published 120 papers in the international journals such as Environmental Science and Technology, Applied Catalysis B: Environmental, Journal of Catalysis, and so on.

For more information, please visit <http://www.scuec.edu.cn/s/277/t/1592/4a/da/info84698.htm>.



**Session B9**

**B39**

**9:15 - 9:40 AM Room B June 22**

## One-dimensional nanoarrays for solar cells

HAO WANG\*

Faculty of Physics and Electronic Science

Hubei University

Wuhan 430062, PR China

Email: nanoguy@126.com

### Abstract

Various kinds of modifying methods towards ZnO and TiO<sub>2</sub> one-dimensional nanostructures such as nanorods and nanotubes have been carried out for their applications in Dye-sensitized solar cell (DSSC), perovskite solar cell (PSC) and photo detectors (PD). Core-sheath ZnO/CdTe and double-sheath ZnO/CdSe/CdTe nanocable arrays as effective photoanode have been developed for solar cells, which resulted in a saturated current as high as 14.3 mA/cm<sup>2</sup>. Large area free-standing highly ordered TiO<sub>2</sub> nanotube arrays on the fluorine-doped tin oxide (FTO) conductive glass substrates have been successfully obtained to serve as photo-anodes of DSSCs. The certified photovoltaic conversion efficiency of TiO<sub>2</sub> nanoarrays based DSSCs is up to 10.3% by using N719 as Dye and I<sup>-</sup>/I<sub>3</sub><sup>-</sup> as electrolyte. Perovskite solar cell with efficiency of up to 18.6% based on TiO<sub>2</sub> nanorod arrays is also presented. Self-powered broadband photodetectors based on CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/ZnO nanorod arrays heterostructure have been achieved with high detectivity of  $3.56 \times 10^{14}$  cm Hz<sup>1/2</sup> W<sup>-1</sup> and high responsivity of 24.3 A W<sup>-1</sup>.

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**Hao Wang** is Professor of Materials Science and Engineering and Vice Dean of Graduate School of Hubei University. He received his Ph. D from Huazhong University of Science and Technology in 1994. He is a visiting professor of University of Cambridge and Aalto University. He has published over 150 refereed journal papers (such as *Adv. Energy Mater.*, *ACS Nano*, *Nano Energy*) and held 18 patents. His research interests involve solar cells, fuel cells, non-volatile memory, photodetectors and magnetic nanostructures.



**Session B9**

**B40**

**9:40 - 10:05 AM Room B June 22**

## Full-spectrum Photocatalysts with Near-infrared Activity

WENXIA LIU, WENWEN GAO, HUABIN CHEN, JUN CHEN

Qilu University of Technology

Jinan, Shandong 250353, China

Email: liuwenxia@qlu.edu.cn

### Abstract

It is in very recently that the investigation of full-spectrum photocatalysts active in near-infrared (NIR) region have gained increasing attention. The strategies for developing an full-spectrum photocatalyst with NIR-activity generally include combination of up-conversion fluorescent materials with semiconductors [1], sensitization with NIR responsive dyes [2], introduction of defect bands, vacancies and the other photosensitive sites into semiconductors for increasing adsorption of NIR light [3,4], application of narrow band gap semiconductors [3] or combination of narrow band gap semiconductors with broad band semiconductors or noble metals [5] for extending absorption edges to NIR light region. Herein we introduced the full-spectrum photocatalysts developed in our research group and analyzed their fabrication approaches for producing NIR photoactivity. Tetragonal  $\beta$ - $\text{In}_2\text{S}_3$  nanoparticle synthesized though a simple hydrothermal method by using sodium sulphate as sulphur source was the first full-spectrum photocatalyst with NIR photoactivity developed in our research group. It shows much higher photocatalytic activity in degradation of methyl orange (MO) in all tested UV, visible and NIR regions. The high photocatalytic activity is attributed to its narrow band gap (1.77 eV), defect spinel structure and sulfur vacancies on the particle surfaces allowing for absorption of NIR light and efficient separation of photogenerated electron-hole pairs [3]. To further corroborating the full-spectrum photocatalytic activity of  $\beta$ - $\text{In}_2\text{S}_3$ , three  $\text{In}_2\text{S}_3$  nanomaterials with different morphology were prepared by using sodium sulphide ( $\text{Na}_2\text{S}$ ), thiosemicarbazide (TSC) and thioacetamide (TAA) as sulphur sources, respectively. All the as-prepared  $\text{In}_2\text{S}_3$  nanomaterials were found to perform well in photodegradation of MO under either UV, visible or NIR light irradiation. The  $\text{In}_2\text{S}_3$  nanomaterial with irregular and plate-like nanoparticles synthesized by using  $\text{Na}_2\text{S}$  as sulfur source shows the best performance due to its exposure of more photoactive (311) plane than the other two  $\text{In}_2\text{S}_3$  nanomaterials and the occurrence of lattice oxygen. The nanomaterials that synthesized by using TSC and TAA as sulfur sources possess the morphology of hollow microspheres, which are hierarchically constructed by thinner nanosheets and cumulated by thicker platelets, respectively. The microsphere sample constructed by thinner nanosheets shows even lower photocatalytic activity than that accumulated by thicker platelets under all the tested light regions especially under longer irradiation time because of its less exposed (311) plane and lower sulfur vacancies although it possesses a far larger specific surface area than the latter [6]. The second full-spectrum photocatalyst active in NIR region is an  $\text{Er}^{3+}$ -doped  $\text{ZnO-CuO-ZnAl}_2\text{O}_4$  multi-phase oxides which was prepared by calcination of  $\text{Zn/Cu/Al/Er}$ -layered double hydroxide ( $\text{Zn/Cu/Al/Er-LDH}$ ). The as-prepared full-spectrum photocatalyst inherited a platelet structure from  $\text{Zn/Cu/Al/Er-LDH}$  and mainly consists of  $\text{Er}^{3+}$ -doped  $\text{ZnO}$ ,  $\text{Er}^{3+}$ -doped  $\text{ZnAl}_2\text{O}_4$  and  $\text{Er}^{3+}$ -doped  $\text{CuO}$  nanoparticles

These metal oxides occur as a commensal that displays a very stable photocatalytic activity over the full solar light spectrum. Compared with the control photocatalyst ZnO-CuO-ZnAl<sub>2</sub>O<sub>4</sub> multi-phase oxides, which was prepared by calcination of Zn/Cu/Al-LDH and also found to possess broad-spectrum photocatalytic activity, the Er<sup>3+</sup>-doped ZnO-CuO-ZnAl<sub>2</sub>O<sub>4</sub> multi-phase oxides display a much better photoactivity in the entire UV and visible regions, and particularly in the NIR region. The excellent photocatalytic activity of Er<sup>3+</sup>-doped ZnO-CuO-ZnAl<sub>2</sub>O<sub>4</sub> multi-phase oxides in the NIR region is ascribed to its Er<sup>3+</sup>-doped CuO-involved multi-crystalline phase heterostructure and the lattice Er<sup>3+</sup> doping-induced distortion, which does not only offer an enhanced NIR absorption but also promotes the separation of photogenerated electron-hole pairs. The third full spectrum photocatalyst we developed is ZnO/ZnFe<sub>2</sub>O<sub>4</sub> photo-Fenton-like catalyst. The ZnO/ZnFe<sub>2</sub>O<sub>4</sub> nanocomposite was prepared by a co-precipitation method followed by calcination. As revealed by optical absorption analysis, the ZnO/ZnFe<sub>2</sub>O<sub>4</sub> nanocomposite exhibits significant optical absorptions in UV, visible and NIR light regions. Benefitting from this unique photo-absorption property and the generation of reactive •OH mainly by the reaction of photogenerated electrons with H<sub>2</sub>O<sub>2</sub>, the ZnO/ZnFe<sub>2</sub>O<sub>4</sub> nanocomposite can degrade MO in the presence of H<sub>2</sub>O<sub>2</sub> under either UV, visible or NIR irradiation. Moreover, the UV, visible and NIR photocatalytic activities of ZnO/ZnFe<sub>2</sub>O<sub>4</sub> nanocomposite are not changed significantly after three runs of recycling [7]. The fourth full-spectrum photocatalyst we developed is TiO<sub>2</sub>/H<sub>2</sub>O<sub>2</sub> thermally-assisted photocatalytic system, in which the presence of H<sub>2</sub>O<sub>2</sub> and the elevated temperatures facilitate the production and separation of electrons and holes, accelerate the carrier transfer at the TiO<sub>2</sub>-electrolyte interface and promote the production of hydroxyl radicals under infrared lamp irradiation. The TiO<sub>2</sub>/H<sub>2</sub>O<sub>2</sub> thermally-assisted photocatalytic system can efficiently degrade lignin in waste water. Suitably increasing the addition level of H<sub>2</sub>O<sub>2</sub> and raising the temperature significantly improve the degradation rate of lignin. The optimal temperature for the thermally-assisted photodegradation of lignin is 70 °C.

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**Wenxia Liu** is Professor of Qilu University of Technology. She is a member of China Technical Association of Paper Industry.

Her current research interests include paper-based photocatalysis, application of nano-technology in the paper making industry such as nanoparticle stabilized paper sizing emulsions, nanoparticle-based retention technique and sticks' control.



## Session B10

## B41

10:20 - 10:45 AM Room B June 22

## Nanowire-plasmonic photocatalysts and thermal emitters

THANG DUY DAO<sup>1</sup>, TADAAKI NAGAO<sup>1,2</sup>, KAI CHEN<sup>1</sup>, SHATOSHI ISHII<sup>1</sup>, GUI HAN<sup>1</sup><sup>1</sup>International Center for Materials Nanoarchitectonics (MANA),

National Institute for Materials Science (NIMS)

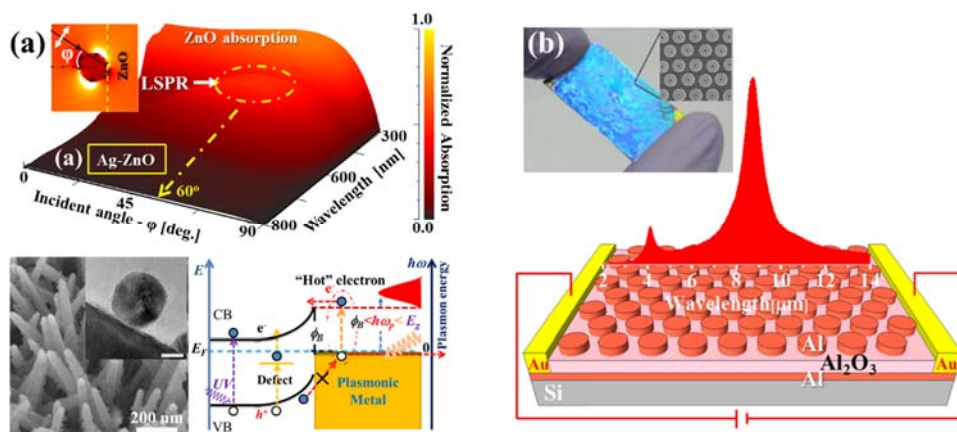
1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

<sup>2</sup>Condensed Matter Physics, Graduate School of Science, Hokkaido University, Kita 8, Nishi 5, Kita-ku, Sapporo 060-0810, Japan.

Email: DAO.Duythang@nims.go.jp; NAGAO.Tadaaki@nims.go.jp

**Abstract**

Optical absorption enhancement using plasmonic structures enables a wide range of applications such as solar energy harvesting devices, light emitting devices and photothermal management. For example, in plasmonic photocatalysis, it has recently attracted great interest in enhancing photocatalytic efficiency not only by the plasmon-enhanced near field but also by the plasmon-enhanced hot-carrier injection, which could boost the visible response of wide bandgap photocatalysts [1]. Here we report measurements and simulations of the efficient sunlight-driven and visible-active photocatalysts composed of plasmonic metals and ZnO nanowire (NW) arrays fabricated via an all-wetchemical route (Fig. 1a) [2]. Another application of plasmon-enhanced light absorption is the perfect absorber and thermal emitter [3]. It is found that with proper designs supported by the electromagnetic simulation, the plasmonic structures could exhibit near perfect absorption at desired resonant wavelengths, making them promising for a number of potential application such as thermal emitters (Fig. 1b) [4], molecular sensors [5] and IR sensors [6].



**Fig.1** (a) Plasmon-mediated photocatalytic activity of ZnO NWs. (b) Plasmonic absorbers for thermal emitters

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**Thang Duy Dao** has been working at the Institute of Physics, Vietnam Academy of Science and Technology (VAST). He received his doctor degree in materials science from Nara Institute of Science and Nanotechnology (NAIST) in 2015. He is currently a JSPS postdoctoral fellow at the Photonics Nano-Engineering Group led by Prof. Tadaaki Nagao in the National Institute for Materials Science (NIMS).

His current research interests focus on design, simulation and fabrication of plasmonic structures for applications in energy conversion and sensing devices.





**Session B10**

**B42**

**10:45 - 11:10 AM Room B June 22**

## Van der Waals Oxide Heteroepitaxy for Transparent and Flexible Electronics

YING-HAO CHU

National Chiao Tung University, Department of Materials Science & Engineering

1001 University Road, Engineering Building 6, R318, Hsinchu 30010, Taiwan

Email: yhc@nctu.edu.tw

### **Abstract**

In the diligent pursuit of low-power consumption, multifunctional, and environmentally friendly electronics, more sophisticated requirements on functional materials are on demand. For example, flexible electronics represents a fast-developing field and has a great potential to impact our daily life. In building up flexible electronics, the materials with controllable conduction, transparency, and good flexibility are required. Recently, the discovery of free-standing 2D materials has created a revolution to this field. Pioneered by graphene, these new 2D materials exhibit abundant unusual physical phenomena that is undiscovered in bulk forms. In the meantime, it also possesses very high transparency to the visible light. However, the extensively studied pristine graphene naturally has no bandgap and become restricted in many field-effect based applications. Hence, looking for various types of new 2D materials has been a focal research direction nowadays. In this talk, we intend to take the same concept, but to integrate a family of functional materials in order to open new avenue to flexible electronics. Due to the interplay of lattice, charge, orbital, and spin degrees of freedom, correlated electrons in oxides generate a rich spectrum of competing phases and physical properties. However, a generic approach to build up flexible electronics based on functional oxides is yet to be developed. In this study, we use a 2D material as the substrate. And we take several functional oxides as model systems, including transparent conducting oxides, VO<sub>2</sub>, NiO, Fe<sub>3</sub>O<sub>4</sub>, Pb(Zr,Ti)O<sub>3</sub>, and oxide nanocomposites, to demonstrate a pathway to build up functional oxides for transparent and flexible electronics.

**Ying-Hao Chu** received his PhD in the Department of Materials Science & Engineering from National Tsing-Hua University in 2004. Then, he joined University of California, Berkeley as a postdoc. In 2008, he acquired an assistant professorship in the Department of Materials Science & Engineering at National Chiao Tung University. In 2013, he started an adjunct position in institute of physics, Academia Sinica. In 2014, he holds an adjunct position in the Department of Electrophysics, National Chiao Tung University. In 2016, he started the adjunct positions in the Material and Chemical Research Laboratories, Industrial Technology Research Institute and the International College of Semiconductor Technology at National Chiao Tung university. His research is highly focused on complex functional oxides and strongly correlated electron systems. He has extensive experience in the use of advanced characterization techniques to understand and manipulate functional oxide heterostructures, nanostructures, and interfaces. His current goal is try to create a pathway to use high quality oxide heteroepitaxy for soft technology. Now, he is a pioneer with the most publication along this research direction.



For more information, please visit <https://sites.google.com/g2.nctu.edu.tw/yhchu>

Session B10

B43

11:10 - 11:35 AM Room B June 22

## N-doped graphene as highly-catalytic counter electrode in Dye-sensitized Solar Cells (DSSCs)

PENG ZHAI

School of Science, Northwestern Polytechnical University, Xi'an, 710072, P. R. China

Email: zhaipeng@nwpu.edu.cn

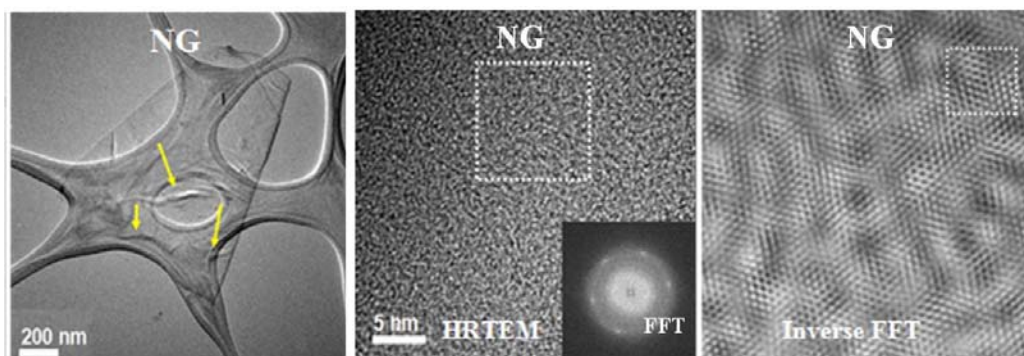
SHIEN-PING FENG

Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Rd., Hong Kong

Email: hpfeng@hku.hk

### Abstract

A significant improvement in efficiency is achieved for Ru-based and porphyrin (YD2-o-C8) based dye-sensitized solar cells (DSSCs), coupled with  $I_3^-/I^-$  and  $[Co(bpy)_3]^{3+/2+}$  mediator electrolyte, respectively. However, the poison of the counter electrode (CE) by the  $[Co(bpy)_3]^{3+/2+}$  mediator remains a significant barrier to producing a reliable high-performance device. In our study, nitrogen-doped graphene nanosheets (NG) are produced using a low cost solution-based process and used as the CE for DSSCs (in **Figure 1**). These produce significantly better electrocatalytic activity than the commonly used Pt CE. The superior performance is a result of the increased number of catalytic sites and the wettable surface that is caused by the substitution of pyridinic and pyrrolic N into the carbon conjugated lattice. We found that the control of the air exposure time after completing N-MEG film is crucial to obtain a reliable NG CE. To the authors' best knowledge, the significantly improved cycling stability (>1000 times) of NG CE for  $[Co(bpy)_3]^{3+/2+}$  redox complexes is demonstrated for the first time.



*Fig.1 HRTEM image of N-MEG nanosheet.*

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**Peng Zhai** is associate professor in the department of applied chemistry, Northwestern Polytechnical University.

His current research interests include Graphene electrodes, Perovskite Solar Cells, and Dye-sensitized Solar Cells.



**Session B10**

**B44**

**11:35 - 12:00 PM Room B June 22**

## **CO<sub>2</sub> Photocatalytic Reduction over TiO<sub>2</sub> Nanocrystals with Coexposed {001} and {101} Facets**

YONGCHUN ZHAO<sup>1</sup>, ZHUO XIONG, ZE LEI, JUNYING ZHANG, CHUGUANG ZHENG

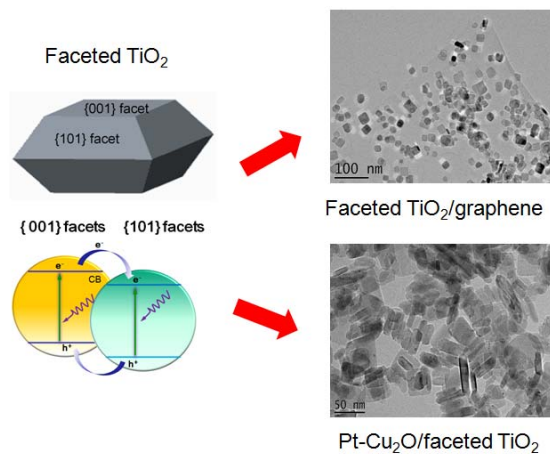
Huazhong University of Science and Technology

Luoyu Road 1037, Wuhan, China

Email: yczhao@hust.edu.cn

### **Abstract**

CO<sub>2</sub> photocatalytic reduction with water is one of the most popular and challenging technologies to produce renewable energy. Engineering TiO<sub>2</sub> with coexposed {001} and {101} facets could enhance the conversion efficiency of CO<sub>2</sub> due to the effective separation of photogenerated charges caused by the formation of {001}/{101} surface heterojunction. However, faceted TiO<sub>2</sub> nanocrystals still suffers from low conversion efficiency and low selectivity for CO<sub>2</sub> reduction. In this paper, faceted TiO<sub>2</sub> nanocrystals were combined with graphene and metal nanoparticles respectively to improve the activity and selectivity of CO<sub>2</sub> photocatalytic reduction. The results show that the faceted TiO<sub>2</sub>/graphene composites exhibited higher CO yield than that of pristine TiO<sub>2</sub> due to the formation of {001}/{101} surface heterojunction and supporting of graphene, which can effectively promote the spatial separation of photogenerated electrons and holes. Differing from graphene, Pt loading tended to promote the production of CH<sub>4</sub> and H<sub>2</sub> while Cu<sub>2</sub>O suppressed H<sub>2</sub> evolution and exhibited lower CH<sub>4</sub> selectivity comparing with Pt. Furthermore, when Pt and Cu<sub>2</sub>O were co-deposited on TiO<sub>2</sub> crystals, H<sub>2</sub> and CO production were both inhibited and CO<sub>2</sub> was selectively reduced to CH<sub>4</sub>. Pt could not only capture photogenerated electrons but also increase the electrons density on the surface of TiO<sub>2</sub>. Meanwhile, Cu<sub>2</sub>O loading enhanced the CO<sub>2</sub> chemisorption on TiO<sub>2</sub> while inhibited that of water. As a result, Pt and Cu<sub>2</sub>O co-deposited TiO<sub>2</sub> crystals exhibited high selectivity for CH<sub>4</sub> production.



**Fig.1** Schematic diagram of graphene and metal modified faceted  $\text{TiO}_2$  nanocrystals

**Yongchun Zhao** is Associate Professor of Energy and Environmental Engineering and Vice Director of State Key Lab of Coal Combustion, Huazhong University of Science & Technology, Wuhan, China. He is a Member of RSC, ACS and TSOP. He was the recipient of the Guangdong Province Science and Technology Progress Award for his contributions to the field of pollutant control from coal-fired power plant in 2015.



His current research interests include CO<sub>2</sub> conversion and utilization; Hg emission and control; mineral transformation and ash deposition; fly ash characteristic and utilization.

For more information, please visit <http://combustion.energy.hust.edu.cn/Data/View/129>.



**Session B11**

**B45**

**14:00 - 14:25 PM Room B June 22**

## Albumin-mediated Gold/Platinum Nanocomposites for Dual Mode CT/MR

### Imaging Applications

WENJING ZHAO, ZHIMING WANG, ZHONGYUN CHU, NENGQIN JIA\*

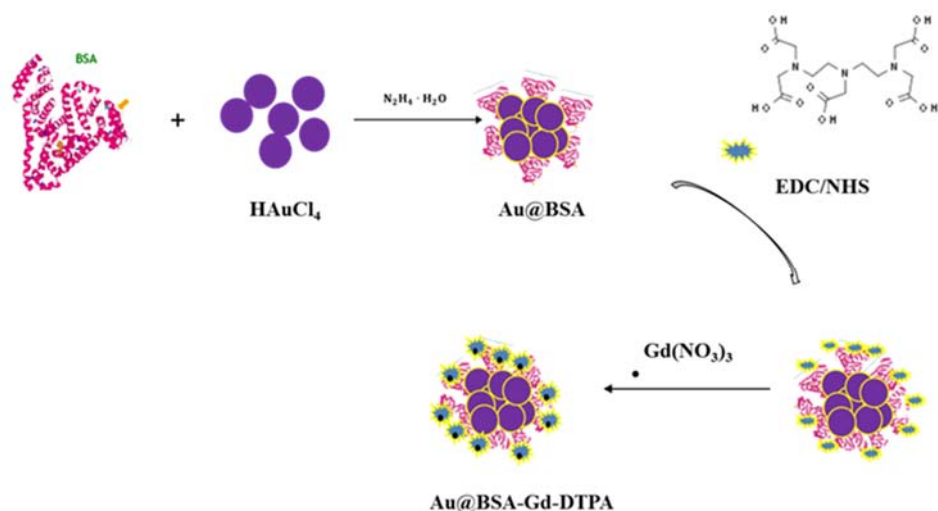
Shanghai Normal University

No.100, Guilin Road, Shanghai, China

Email: nqjia@shnu.edu.cn

#### Abstract

Contrast agents play a vital role in the enhanced examination of biomedical imaging. However, traditional clinical small-molecule agents face a variety of drawbacks, such as low blood circulating time, difficult modification and potential toxic and side effects. Herein, a simple albumin directed fabrication of gold (Au) or platinum (Pt) nanoparticles was achieved for exploring the utilization in CT and MR imaging. Firstly, ultra-small nanoagents (Pt@BSA) with a mean core size of 2.1 nm were obtained through a facile one-pot synthesis by the reduction of chloroplatinic acid hexahydrate using bovine serum albumin (BSA) as the biotemplate under room temperature. It was demonstrated that the nanocrystals could serve as potential new and potent CT contrast agents, especially vital for in vivo imaging with prominent enhancement and metabolizable behaviours due to the combination of the higher X-ray attenuation property and prolonged imaging time [1]. Then gold nanoparticles (Au@BSA) were also prepared with BSA as a biotemplate following with conjugation of diatrizoic acid (DTA) for a potential CT imaging contrast agent (Au@BSA-DTA). The biomimetic material Au@BSA-DTA with double radiodense elements of Au and iodine displayed much stronger CT imaging effect compared with the traditional small molecule contrast agents [2]. Finally, a novel CT/MR contrast agent Au@BSA-Gd-DTPA was fabricated by modifying the as-prepared Au@BSA with diethylene triamine pentaacetic acid (DTPA), followed by the chelation of Gd (III) ions. For the CT phantoms, the formed nanocomplex showed an improved contrast in CT scanning than that of Au@BSA as well as small molecule iodine-based CT contrast agents, and for the T<sub>1</sub>-weighted MRI images, the nanoagents displayed a relatively higher  $r_1$  relaxivity than that of the commercial MR contrast agents. Importantly, the above mentioned nanoagents exhibited not only good colloid stability and water dispersibility, but also satisfying low-cytotoxicity and hemocompatibility. In summary, we have constructed a series of novel biomaterials that can be used as contrast agents for both X-ray CT and MR phantoms, which paves the potential clinical applications in cancer early diagnosis.



**Fig.1** A schematic illustration of the preparation of the Au@BSA-Gd-DTPA.

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**Nengqin Jia** is a Professor of Chemistry at Shanghai Normal University. He has published over 60 papers in refereed journals (e.g. *Nano. Lett.*, *J. Am. Chem. Soc.*, *Anal. Chem.*) and has been one of Editorial Board members of *Nano Biomedicine and Engineering*. He has been awarded as Shanghai Rising Star, New Century Excellent Talent of Ministry of Education and Shanghai Shuguang Scholar.



His current research interests include nanobiotechnology, biosensors, and bioelectrochemistry.

Session B11

B46

14:25 - 14:50 PM Room B June 22

## Manganese oxide-embedded iron oxide nanoparticles: An enhanced $T_1$ - $T_2$ dual-modal contrast agent

CHICHONG LU<sup>1,2\*</sup>, JIANMEI MA<sup>1</sup>

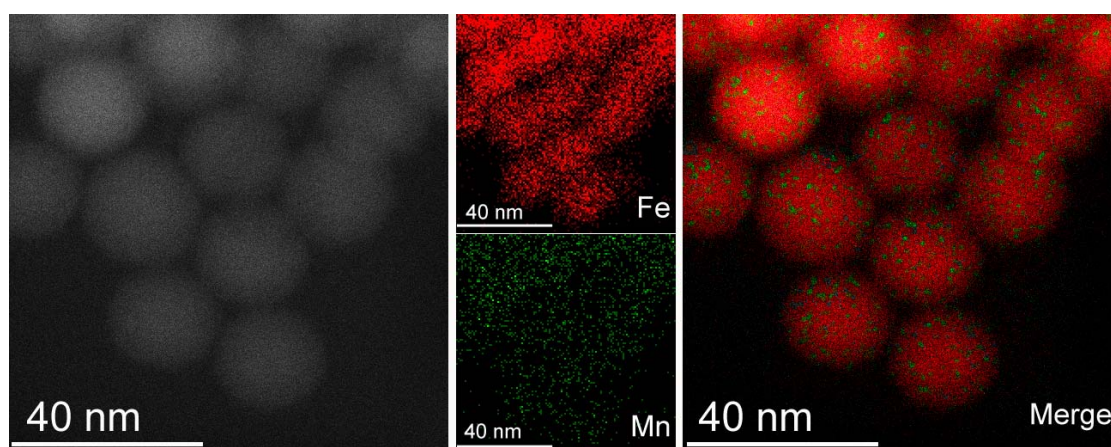
<sup>1</sup> Department of Chemistry, School of Science, Beijing Technology and Business University  
Beijing 100048, P. R. China

<sup>2</sup> Key Laboratory of Cosmetic, China National Light Industry, Beijing Technology and Business University  
Beijing 100048, P. R. China

Email: luchichong@btbu.edu.cn

### Abstract

The  $T_1$ - $T_2$  dual-modal magnetic resonance imaging (MRI) contrast agents can greatly improve the sensitivity and reliability by the beneficial contrast effects in both  $T_1$  imaging with high tissue resolution and  $T_2$  imaging with high feasibility on detection of a lesion. We report a facile one-pot synthesis of manganese oxide-embedded iron oxide ( $\text{Fe}_3\text{O}_4/\text{MnO}$ ) nanoparticles by thermal decomposition of iron-oleate and manganese chloride. The Mn/Fe molar ratios in the final nanoparticles can be well tuned by the Mn/Fe molar ratios in the reaction precursors. After PEG-phosphate coating,  $\text{Fe}_3\text{O}_4/\text{MnO}$  nanoparticles significantly increase the  $T_1$  relaxivity with an enhanced positive contrast effect. Moreover, both  $r_1$  and  $r_2$  values of  $\text{Fe}_3\text{O}_4/\text{MnO}$  nanoparticles can be tuned by varying Mn/Fe ratios. Therefore, the facile synthetic method and surface coating strategy, and the highly biocompatibility of  $\text{Fe}_3\text{O}_4/\text{MnO}$  nanoparticles promise the potential biomedical applications in MR imaging.



**Fig.1** TEM image with high angle annular dark field and EDX mapping images of  $\text{Fe}_3\text{O}_4/\text{MnO}$  nanoparticles.

**References**

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**Chichong Lu** is associate Professor of Chemistry at Beijing Technology and Business University and Director of Department of Chemistry. He graduated from Nanjing Tech University with a BS and received his PhD from Wonkwang University.

His current research focuses on synthesis and interfacing inorganic nanocrystals with biological systems using chemical means for MRI-based molecular imaging and biosensors.



**Session B11**

**B47**

**14:50 - 15:15 PM Room B June 22**

## Tracking of Stem Cells with Magnetic Resonance Imaging

QUN ZHAO

Bioimaging Research Center & Department of Physics

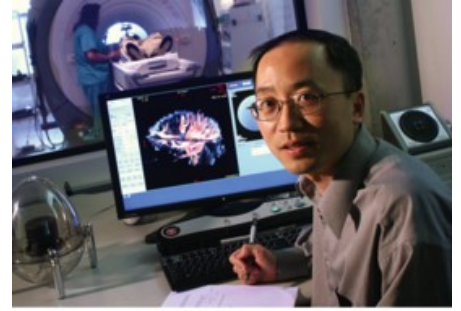
University of Georgia, Athens, GA., USA

Email: qzhao@physast.uga.edu

### **Abstract**

Recently various cell therapies have improved outcome of many diseases. A critical component of cell therapies is the ability to track the cells after transplantation. Monitoring a cell's survival, migration, differentiation, and integration within host tissue is crucial for assessing the safety and efficacy of cellular treatments. In this talk magnetic resonance imaging (MRI) based tracking of stem cells is presented, where cells labeled with superparamagnetic iron oxide (SPIO) nanoparticles can be tracked in a chicken embryo model up to 10 days post transplantation. Nevertheless, SPIO nanoparticles as a  $T_2^*$  contrast agent are usually associated with signal loss in MR images, leading to difficulties for cell tracking. To overcome this problem, a new imaging sequence, SWIFT with water and fat suppression, is introduced. Compared with other conventional pulse sequences, such as spin echo and gradient-recalled echo, the SWIFT approach enhances in vivo mapping of SPIO distribution in tissues, and improves detection sensitivity of SPIO nanoparticles.

**Qun Zhao** is an Associate Professor of Physics and Director of Magnetic Resonance Imaging Lab, University of Georgia. He is a senior member of IEEE, and a Member of International Society of Magnetic Resonance in Medicine. His current research interests include magnetic resonance imaging, applications of magnetic nanoparticles in MRI, and machine learning. For more information, please visit <http://www.physast.uga.edu/~qzhao/>.





Session B11

B48

15:15 - 15:40 PM Room B June 22

## Surface Passivation of Magnetic Nanoparticles via Atomic Layer Deposition

RONG CHEN

Huazhong University of Science and Technology

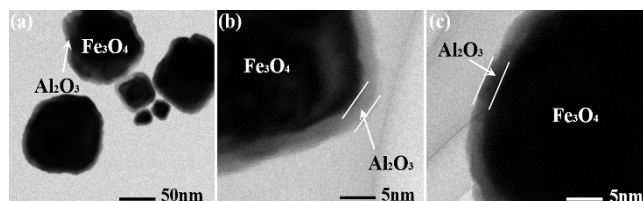
1037 Luoyu Road, Wuhan, P.R.China

Email: rongchen@hust.edu.cn

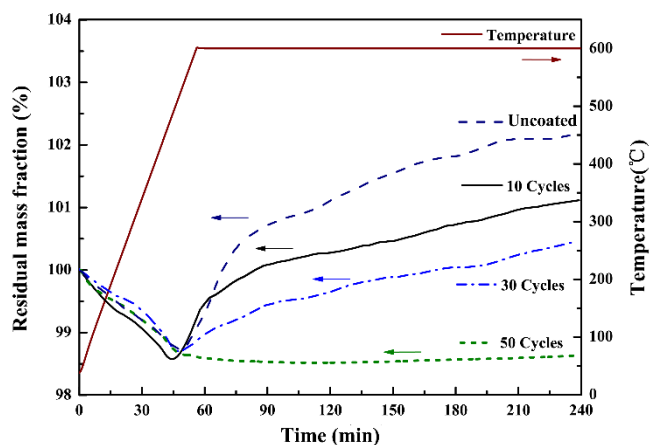
### Abstract

Iron(II,III) oxide ( $\text{Fe}_3\text{O}_4$ ) as a typical magnetic material, have received great attention for applications, including magnetic resonance imaging (MRI), biochemical sensing, hyperthermia treatment, targeted delivery of pharmaceuticals and therapeutic genes.[1] One of the obstacles for these applications, is the tendency of these nanoparticles towards oxidation and magnetization loss under ambient conditions. The  $\text{Fe}_3\text{O}_4$  nanoparticles often oxidize to  $\text{Fe}_2\text{O}_3$  spontaneously and consequently suffer a loss of magnetization.[2] An effective way to overcome this obstacle is to passivate the surface of  $\text{Fe}_3\text{O}_4$  nanoparticles to prevent ambient oxygen reaction.

Atomic layer deposition (ALD) is an attractive technique to deposit ultrathin nanoscale films onto high-aspect-ratio surfaces and afford precise thickness control at atomic scale.[3] In this work, a home-built rotating fluidized bed atomic layer deposition reactor was employed to form dense and uniform ultrathin layer of oxide passivation layers on  $\text{Fe}_3\text{O}_4$  nanoparticles.[4] Uniform passivation layers around the magnetic cores were demonstrated by both transmission electron microscopy and the statistical analysis of Al mass concentrations. Individual particles were coated instead of the soft agglomerates, as was validated by the specific surface area analysis and particle size distribution. Alumina has been chosen as a representative coating materials owing to its good stability and biocompatibility, its high efficiency for oxidation resistance, and process ease for ALD.[5] The results of thermogravimetric analysis suggested that  $\sim 5$  nm  $\text{Al}_2\text{O}_3$  coatings as shown in Fig 1.could effectively protect the  $\text{Fe}_3\text{O}_4$  nanoparticles from oxidation (Fig. 2). The X-ray diffraction patterns also showed that the magnetic core crystallinity of such passivated nanoparticles could be well preserved under accelerated oxidation conditions. The precise thickness control via ALD maintained the saturation magnetization at 66.7 emu/g with a 5 nm-thick  $\text{Al}_2\text{O}_3$  passivation layer. This good preservation of the magnetic properties with superior oxidation resistance will be beneficial for practical MRI as well as other magnetic-based applications.



**Fig.1** TEM images in bright field of 5nm  $\text{Al}_2\text{O}_3$  coated  $\text{Fe}_3\text{O}_4$  nanoparticles



**Fig.2** TG curves of bare and different cycles  $Al_2O_3$  coated  $Fe_3O_4$  nanoparticles

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**Rong Chen** is a professor in School of mechanical science and engineering, School of optical and electronic information by courtesy, Huazhong University of Science and Technology (HUST). She is also an adjunct professor, Ningbo Institute of materials technology and engineering, Chinese Academy of Sciences (CAS).



She received her Doctoral and Master degrees from Stanford University and bachelor degree from University of Science and Technology of China (USTC). She joined school of mechanical science and engineering, Huazhong University of Science and Technology in 2011. Prior to that, she was a senior research scientist in Intel Labs and Applied Materials, Inc., Santa Clara, USA performing research and development in VLSI process and related equipment development. She is the recipient of “Young and middle-aged leading scientists, engineers and innovators” by ministry of science and technology of China, “the Recruitment Program of Global Young Experts” of The Organization Department of the Central Committee of the CPC, “New Century Excellent Talents in University” of the Ministry of Education, “Distinguished Young Talents of Hubei Province”. She is also the recipient of the Simon Karecki award of Semiconductor Research Association, the Texas Instruments Graduate Woman’s Fellowship for Leadership in Microelectronics, China Overseas innovation talents contribution award, Geneva international innovation exhibition Gold award, and so on.

Prof Chen’s research is focused on the fabrication, design and properties of ultrathin films and nanostructures, and applying to a range of problems in sustainable energy and environment, semiconductor processing, flexible displays, MEMS/NEMS, and nanotechnology. These new interdisciplinary fields in nanoscience and nanotechnology supersede the more traditional disciplines and demand new paradigms for collaboration. Her current research areas include: 1)Developing highly engineered inorganic nanostructures with well-defined chemical composition, physical dimension and structure, and assembly of them into increasingly complex architecture 2)Investigating fundamental properties of such materials and exploring them as functional nano-systems for applications in electronics, optoelectronics, and sustainable energy 3)Fundamental understanding of such materials properties through the combination of experimental and theoretical modeling, and provide means of rational design of experiments 4)Design equipment apparatus to achieve the above fabrication goals based on different applications and their requirements.

For more information, please visit <http://english.mse.hust.edu.cn/faculty/directory-detail/840>; and <http://www.materialssimulation.com/>

Session B12

B49

16:00 - 16:25 PM Room B June 22

## Proteins promote cancer nanotheranostics

BINGBO ZHANG

The Institute for Biomedical Engineering & Nano Science, Tongji University School of Medicine, Shanghai, 200443, China

Email: bingbozhang@tongji.edu.cn

### Abstract

Utilizing molecular imaging probes can increase the detection rate and diagnosis accuracy of tumors. However, the non-specific adsorption of nanoprobe is seriously affecting the detection accuracy and sensitivity. Leveraging on the unique domains and amino acid sequences of bio-endogenous proteins, some specific tactics, including surface engineering of nanoparticles with proteins, and protein-mediated biomimetic synthesis of nanoprobe have been developed in a green chemistry fashion in our group [1~4]. This protein-mediated cancer nanotheranostic strategy is of great significance in reducing nonspecific adsorption of nanoprobe for in vitro diagnosis and in vivo applications. Capitalizing on this strategy, protein-coated nanoparticles with single-/dual- imaging modality were fabricated. Furthermore, therapeutical moieties can be imparted to the above structures in a one-pot manner for enhanced tumor theranostics. Particularly, the operating mechanisms of these reactions are preliminarily studied [5].

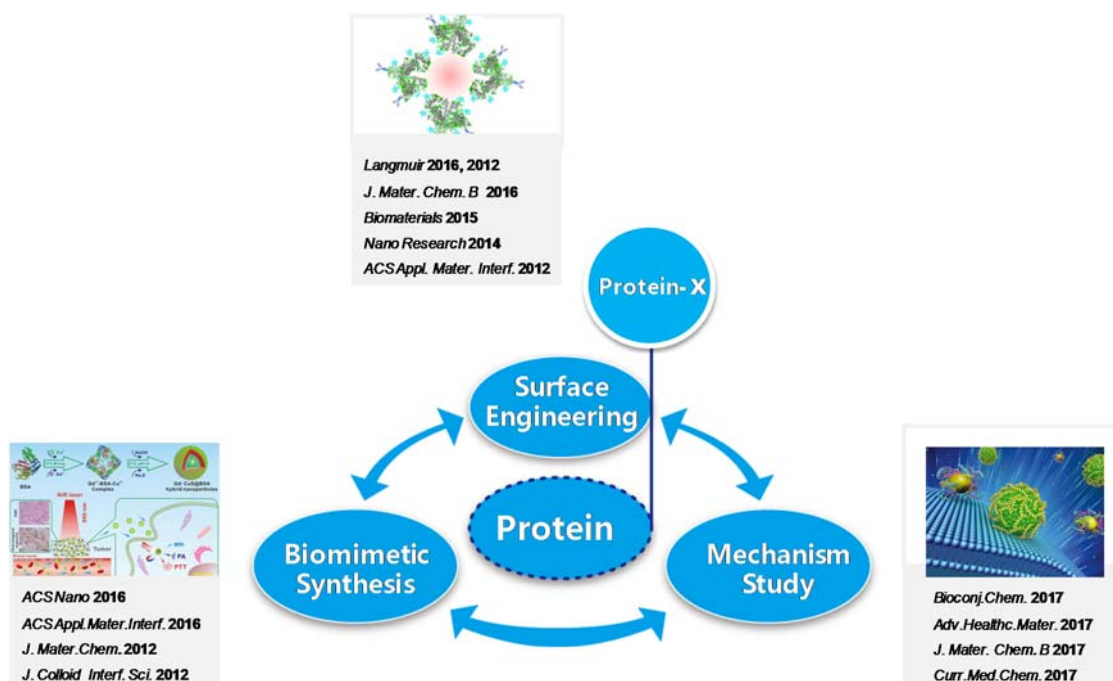


Fig.1 Protein-Mediated Biomimetic Tactics in Our Group.

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**Bingbo Zhang** started his research career in the School of Medicine at Tongji University in 2009 as an Assistant Professor. Currently he is an Associate Professor in the School of Medicine, and a Principal Investigator in the institute of photomedicine of Tongji University School of Medicine. Dr. Zhang is the member of youth committee of Chinese Society of Biomedical Engineering (CSBE), Chinese Society of Particuology (CSP), and Chinese Optical Society (COS). Dr. Zhang has published over 40 peer-refereed journal papers, including ACS Nano, Biomaterials, Theranostics, Adv. Healthcare Mater., Bioconjugate Chem., Langmuir, etc., with an h-index of 15.



His current research interests include biomaterials, nanomedicine, and in vitro diagnosis.

For more information, please visit [http://inano.tongji.edu.cn/html/people/dr\\_bingbo\\_zhang.html](http://inano.tongji.edu.cn/html/people/dr_bingbo_zhang.html).

**Session B12**

**B50**

**16:25 - 16:50 PM Room B June 22**

## Nanoparticles in Magnetic Resonance Imaging

RENHUA WU, ZHIWEI SHEN, ZHUOZHI DAI

Department of Medical Imaging, Shantou University Medical College

22 Xinling Road, Shantou 515041, China

Email:

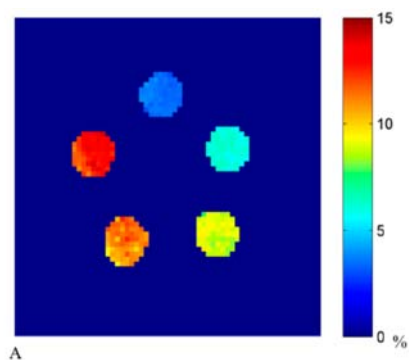
Renhua Wu rhwu@stu.edu.cn

Zhiwei Shen zwshen@stu.edu.cn

Zhuozhi Dai zzdai@163.com

### **Abstract**

Magnetic resonance imaging (MRI) provides crucial roles in diagnosis and treatment of human diseases. More and more new MRI techniques have been developed recently. Among them, chemical exchange saturation transfer (CEST) imaging [Fig1] has shown its promising for noninvasive pH imaging and metabolic imaging. [1] Nanoparticles have also been studied widely in the field of magnetic resonance imaging, including disease detection and stem cell migration. For example, superparamagnetic iron oxide nanoparticles (SPIONs) have been intensively studied for their biomedical applications as T2 contrast agents in MRI. We collaborated with Zhang BL group [2] and found that compared with other nanoparticles, SPIONs exhibit highmagnetic responsivity which can reduce the amount of the contrast agents needed for calcium-responsive MRI, low cytotoxicity, higher biocompatibility and chemical stability. The assessment of changes in the extracellular calcium concentration by magnetic resonance imaging would be a valuable biomedical research tool to monitor brain neuronal activity. The nanoparticles, EGTA-SPIONs, have potential as smart contrast agents for Ca<sup>2+</sup>-sensitive MRI. We also collaborated with Bu WB group [3] and found that both T1-weighted imaging and in vivo pH mapping can be successfully acquired on the kidney and glioblastoma (GBM) of the mouse after intravenous injection of the T1/CEST NaGdF<sub>4</sub>@PLL nanodots (NDs), demonstrating the feasibility of such an anatomical and functional dual-mode imaging technique on one magnetic resonance machine by the rational design of MRI contrast agents. Meanwhile, the PLL shell exhibits a sensitive CEST effect that depends on the pH value of the lesions. Attractively, these ultrasmall nanoagents could be excreted through urine with negligible toxicity to body tissues, which has been demonstrated by the blood biochemistry, hematology, and tissue H&E staining analysis.



**Fig.1** CEST images of creatine tubes of different concentrations.

### References

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**Renhua Wu** is a Professor at Shantou University Medical College. He is a member of IEEE and IEEE Engineering in Medicine and Biology Society (EMBS). Being advised by the world famous radiologist, Prof. Reiser MF, he got his doctor degree from Ludwig Maximilian University of Munich in 1997.

For more information, please visit <http://www.med.stu.edu.cn/jx/ms/info26.asp>.



**Poster Session**

**16:50 - 18:00 PM**

P1

## Two color optical absorption in InAs/AlSb/GaSb quantum well

XIANGFEI WEI

West Anhui University

Email: flyxfwei@sina.com

### **Abstract**

In order to suppress the noise and improve the performance of the detector, the AlSb caplayer is inserted between the InAs layer and GaSb layer. The transfer matrix method is employed to solve the Schrödinger equation to get the wavefunctions and subband energies for electron and hole. The optical absorption coefficients are obtained by solving the Boltzmann equation with the balance equation method. The effects of the AlSb caplayer on the intersubband optical transition are investigated in detail. The noise induced by the electron-hole combination is suppressed efficiently when the width of the AlSb caplayer reaches up to 2 nm. Two peaks of the optical absorption are observed at the Mid-and-far Infrared bandwidth indicating that the InAs/AlSb/GaSb based type II quantum well system can be used as Mid-and-far Infrared photoelectric detector.

**Keywords:** Two color optical absorption, InAs/AlSb/GaSb quantum well, Electron-hole combination noise

**Poster Session**

**16:50 - 18:00 PM**

P2

## Enhanced electrochemical energy storage of N-doped graphene by adsorbing molecules of hydrolyzized polyimide

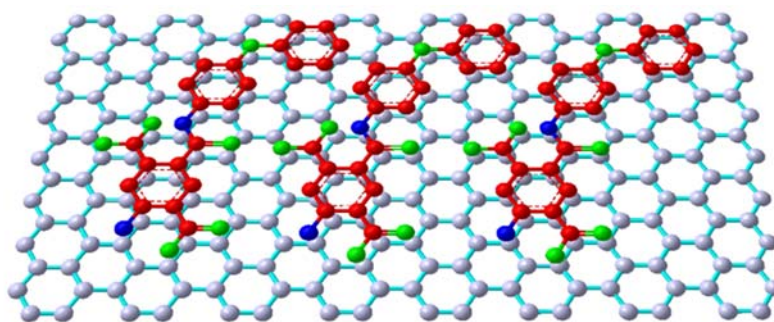
YI ZHAO, JINZHANG LIU

Beihang University, Beijing, 100191, China

Email: ljz78@buaa.edu.cn

### Abstract

A novel approach for increasing the specific capacitance of graphene-based supercapacitors is reported. In this work, Kapton, which is polyimide (PI) film widely used in industry, is used as the starting material to functionalize graphene. Hydrolysis of PI in alkalic solution released small aromatic molecules containing pyrrolic nitrogen that can be dissolved in water and easily adsorbed onto graphene sheets via  $\pi$ - $\pi$  interaction (Fig.1). These small molecules store charge via a redox process, endowing graphene with pseudocapacitance and increasing the specific capacitance. N-doped graphene films are obtained by hydrothermally reducing solid composite films consisting of graphene oxide, ammonium acetate, and salt. These films are firstly used as electrodes to make symmetric supercapacitors with  $\text{H}_2\text{SO}_4$  aqueous electrolyte as electrolyte, and show specific capacitances around 310 F/g. After the adsorption of hydrolyzized PI molecules, the weight of graphene film is  $\sim 3\%$  increased, and the specific capacitance was remarkable increased up to 467 F/g. Notably, the areal specific capacitance is in the scale of  $1.2 \text{ F/cm}^2$ . When using the  $\text{Li}_2\text{SO}_4$  aqueous electrolyte that can extend the potential window to 1.5 V, the device also remains high specific capacitance around 445 F/g, and exhibits high energy densities up to 35 Wh/Kg. Our devices not only deliver excellent capacitive performances in aqueous electrolyte (89% capacitance retention at 20 A/g and 85% capacitance retention over 5 000 cycles), but also exhibit extraordinary mechanical flexibility. This novel strategy by adsorbing small molecules from hydrolyzized PI provides a promising route towards high-performance supercapacitors.



**Fig.1.** Illustration of the adsorption of hydrolyzized PI molecules onto graphene sheet.

**Yi Zhao** is a PhD student at School of Materials Science and Engineering, Beihang University, Beijing, China. Her research interests include the synthesis and functionalization of graphene and other porous carbon materials and their application in supercapacitors.

Email: [by1601141@buaa.edu.cn](mailto:by1601141@buaa.edu.cn)



**Poster Session**

**16:50 - 18:00 PM**

P3

## Gram-scale production of nanoporous graphene by Mg-thermoreduction of CS<sub>2</sub> for electrochemical energy storage

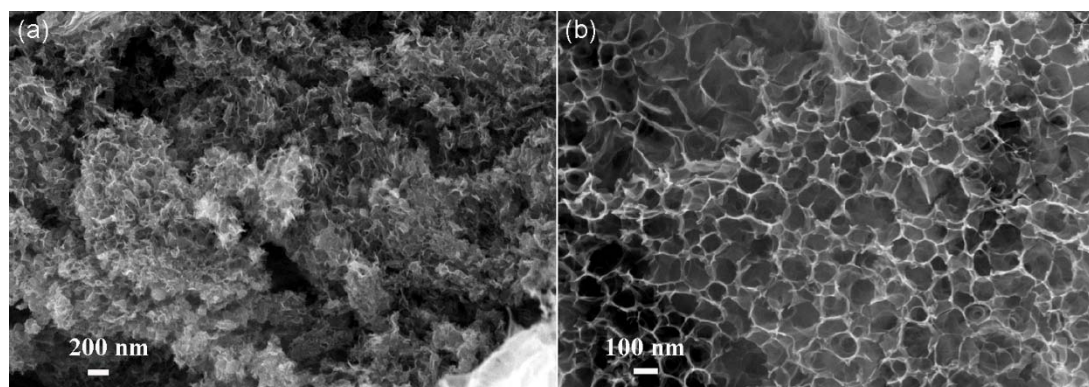
LU SUN, JINZHANG LIU, YAN LI

Beihang University, Beijing, 100191, China

Email: liyan@buaa.edu.cn

### Abstract

Mass production of porous carbon at low cost for supercapacitor applications is highly desired. Herein, for the first time we report a novel method to grow porous 3D graphene by using Mg to reduce CS<sub>2</sub> vapor. In a tube furnace the mixture of Mg and NaCl powders are heated at 570 °C and reacted with CS<sub>2</sub> vapor carried by an Ar flow. The Mg powder can be about 95% consumed and the weight of resultant carbon nanomaterial is in gram scale after one experiment. This 3D graphene product with specific surface area of 980 cm<sup>2</sup>/g is processed into electrodes for electrochemical test, showing a specific capacitance of 212 F/g at 1 A/g in H<sub>2</sub>SO<sub>4</sub> aqueous electrolyte. Besides, the electrode is continuously charged/discharged at 5 A/g for 10,000 cycles and its capacitance remains 98.5% of the original value.



**Fig.1.** (a) and (b) SEM images of the 3D graphene product at low and high magnifications.

**Lu Sun** is currently a Ph.D student in Materials Science at Beihang University, Beijing, China. She received her B.S. and M.S. degrees from Shandong University of Science and Technology, Qingdao, China, in 2012 and 2015, respectively. Her research interests focus on the preparation of graphene and its application in energy storage devices. She has published 1 SCI journal paper and filed 3 patents, in which 1 has been granted.



## Poster Session

16:50 - 18:00 PM

P4

## Novel Self-powered UV-Visible Photodetector with Fast Response and High Photosensitivity Employing Fe:TiO<sub>2</sub>/n-Si Heterojunction

LIN SUN, CHUNRUI WANG

Department of Applied Physics and state key laboratory for modification of chemical fibers and polymer materials, Donghua University,

2999 Renmin Rd North, Songjiang District, Shanghai, P.R.China

Email: suns@mail.dhu.edn.cn, crwang@dhu.edu.cn

TAO JI

State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, College of Materials Science and Engineering, Donghua University

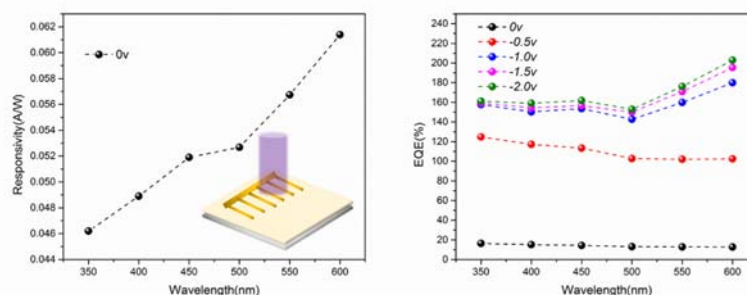
2999 Renmin Rd North, Songjiang District, Shanghai, P.R.China

School of Fundamental Studies, Shanghai University of Engineering Science,

333 Long Teng Road, Songjiang District, Shanghai, P.R.China

### Abstract

A UV-Visible photodetector employing heterojunction between the Fe:TiO<sub>2</sub> and Si was fabricated via a facile solution process. The existence of built-in electric field between TiO<sub>2</sub> and Si help facilitate the separation of photogenerated electron-hole pairs and regulate the electron transport. Under zero bias, the device exhibited high responsivity of 46 mA/W (350 nm) and 60 mA/W (600 nm) with a 0.5 mW·cm<sup>-2</sup> light irradiation. At a small reverse bias of -0.5V, the quantum efficiency of the heterojunction rise up beyond 100% with a broad wavelength range. The exploring of Fe:TiO<sub>2</sub>/n-Si heterojunction photodetector demonstrates an ultrasensitive (on/off ratio up to 10<sup>3</sup>), fast (rise/decay time of <10/15 ms), and broad-band (UV-visible) photodetection with no or low external energy supply. Such novel photodetector with Fe:TiO<sub>2</sub>/n-Si Heterojunction might be potentially useful for relative applications with weak-signal fast detection in UV-visible band.



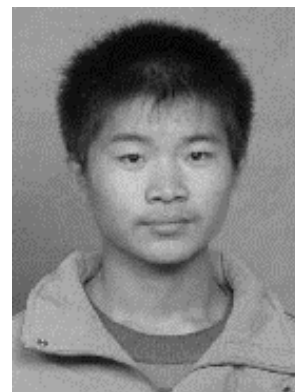
**Fig.1** Responsivity and EQE of Fe:TiO<sub>2</sub>/n-Si heterojunction under each bias in UV-visible band

**References**

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**Lin Sun** is a Ph.D. candidate in Prof. Chunrui Wang's group of Donghua University. His current research interests include low-dimensional inorganic semiconductors and their optoelectronic applications.



## Poster Session

16:50 - 18:00 PM

P5

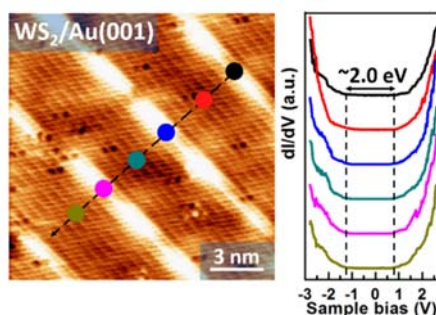
# Quasi-Freestanding Monolayer Striped WS<sub>2</sub> with an Invariable Band Gap on Au(001)

M. HONG, Y. F. ZHANG\*

Department of Materials Science and Engineering, College of Engineering, Peking University  
 Center for Nanochemistry (CNC), Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University  
 No.5 Yiheyuan Road Haidian District, Beijing, P.R. China  
 Email: yanfengzhang@pku.edu.cn

## Abstract

Revealing the structural/electronic features and interface interactions of monolayer MoS<sub>2</sub> or WS<sub>2</sub> on metals is essential to evaluating the performance of related devices. Herein, we focused on the atomic-scale features of monolayer WS<sub>2</sub> on Au(001) derived from the chemical vapor deposition (CVD) synthetic route. The results of scanning tunneling microscopy and spectroscopy (STM/STS) reveal that the WS<sub>2</sub>/Au(001) system possesses a striped superstructure similar to that of MoS<sub>2</sub>/Au(001) and a weaker interfacial interaction, as evidenced by both experimental and theoretical investigations. Specifically, the band gap of WS<sub>2</sub>/Au(001) manifests a relatively intrinsic value of ~2.0 eV. However, the band gap can be gradually decreased to ~1.5 eV by increasing the sample annealing temperature from ~370°C to 720°C. Additionally, the doping level (or Fermi energy) of monolayer WS<sub>2</sub>/Au(001) is nearly unchanged over the valley and ridge regions of the striped patterns, which is explained by the homogenous distributions of point defects introduced by annealing. Briefly, this work provides an in-depth investigation into the interfacial interactions and electronic property of monolayer MX<sub>2</sub> on metal substrates. [1].



**Fig. 1** STM image (0.20 V, 940 pA, 15 × 15 nm<sup>2</sup>) of WS<sub>2</sub>/Au(001) after 2 h of annealing the sample at ~370°C, and the corresponding STS spectra (2.50 V, 200 pA, 10 mV, 932 Hz) at the positions marked with colored dots (along the black arrow).

**References**

- [1] M. Hong, Y. F. Zhang\*, Quasi-Freestanding Monolayer Striped WS<sub>2</sub> with an Invariable Band Gap on Au(001). Nano Research, 2017, Accepted.

**Min Hong** received her B. S. degree in Central China Normal University in 2015. Currently, she is a Ph. D candidate in Department of Materials Science and Engineering, Center for Nanochemistry, Peking University.

Her current research interests include scanning tunneling microscopy/spectroscopy (STM/STS) studying on atomic structures and electronic properties of two-dimensional materials.



**Poster Session**

**16:50 - 18:00 PM**

P6

## Continuous and high-efficient synthesis of graphene oxide based on modified hummers method

XIAOSHAN ZHANG, TIANJIAO HUANG, CHUNYAN ZHOU, YUWEI LAN, GUANGYAO JIA, HONG YANG, YILIN WANG, LIYA ZHOU\*

School of Chemistry and Chemical Engineering

Guangxi University, Nanning, 530004, China

\*Corresponding author: Tel.: 86-771-3236178; Fax: 86-771-3233920.

Email: zhouliyatf@163.com

### **Abstract**

We report a modified Hummers method in which the amount of potassium permanganate was increased while maintaining the thermal cycle of the system. Compared with the traditional Hummers method, it offers easier procedures while producing greater amount of oxygen-containing groups (~30%) at a high yield. The prepared graphene oxide(GO) also exhibited greater layer spacing ( $>0.834$  nm), which is beneficial for the sonication dispersion. Thus, the modified Hummers method shows desirable prospects for large-scale industrial production and applications of GO, in addition to its derivatives and market potential.

**Keywords:** Carbon and graphite; layered structures; Modified hummers method; Raman spectroscopy; X-ray diffraction

**Poster Session**

**16:50 - 18:00 PM**

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## Recent research in the continuous terahertz wave on nondestructive detection of carbon fibre composite

TIELIN LU, CHUNXI WANG

Technology and Economy Institute (Institution)

397A Guanganmenwai St., Beijing, China

Email: lutielin@126.com, wchx@tc124.com

JINGSHUI ZHANG, LINGQIN KONG

Beijing Institute of Technology (Institution)

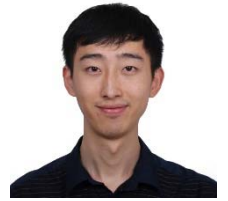
No.5 Zhongguancun South St., Beijing, China

Email: 177345890@qq.com, 4434755558@qq.com

### **Abstract**

Terahertz nondestructive detection system is to test the image of the carbon fibre composite material. We use the continuous back wave oscillator (BWO) to pump the terahertz radiation, which the frequency is range from 210-250 GHz. By the reflection type detection system, the terahertz probe focus moves from the surface of the concealed carbon fibre composite material. In order to get real-time scanning the material image, the material is located by the 2D translation machine, which is connected to the computer. The data is collected by the phase-locked amplifier and calculated by the Matlab using the least square method (LSM). The interior structure, such as cracks, inclusions, empty and bubbles, can be detected by the images nearly 1mm resolution, which is a more convenient and simple method of nondestructive detection of the carbon fiber composite material.

**Dr. Tielin Lu** is Engineer of Standard and Test Center in Instrumentation Technology and Economy. He has got the PHD from Beijing Institute of Technology. He is a Member of National TC124 On Industrial Process Measurement, Control and Automation. He is also the expert of the IEC/TC65/SC65E/WG2.



His current research interests include Optical Instrument, Terahertz Imaging, Laser Physics, and Standard Instrument.

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