



**Nano-Micro  
Conference  
2018  
Conference Program**

December 17-20 2018 Jeju, South Korea



# Conference Program

## Contents

General Information .....	I
Registration Desk Hours .....	V
Conference Venue .....	V
Conference Schedule .....	VI
December 16 .....	VI
December 17, Room A .....	VI
December 17, Room B .....	VIII
December 18, Room A .....	X
December 18, Room B .....	XII
December 18, Room C .....	XIV
December 19, Room A .....	XVI
December 19, Room B .....	XVIII
December 20 .....	XX
Abstracts .....	1
Author Index .....	97

## General Information

**Nano-Micro Conference 2018** 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

Prof. Dr. **Yafei Zhang**

Cheung Kong Scholar

Director, Key Laboratory for Thin Film and Microfabrication Technology of the Ministry of Education

Shanghai Jiao Tong University, China

Editor in Chief of Nano-Micro Letters

Prof. Dr. **Hyoyoung Lee**

Director of Creative Research Institute

SKKU-Fellow Professor of Chemistry, Energy Science and SAINT,

Associate director of Institute for Basic Science-Center for Integrated Nanostructure Physics

Sungkyunkwan University, Republic of Korea

### Advisory Committee Chair

**Ben Zhong Tang**, Member of Chinese Academy of Sciences, The Hong Kong University of Science & Technology, Hong Kong SAR

### Scientific Program Committee Chair

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

### Organizing Committee Chair

**Giovanni Benelli**, University of Pisa, Italy

### Workshop Chair

**Saskia F. Fischer**, Humboldt-Universität zu Berlin, Germany

**Katsuhisa Taguchi**, Kyoto University, Japan

**Arun Bansil**, Northeastern University, USA

**Sang-Yong Ju**, Yonsei University, Republic of Korea

**Ray Chen**, The University of Texas, USA

**Xinhua Qi**, Agro-environmental Protection Institute, China

**Liwen Sang**, National Institute for Materials Science (NIMS), Japan

**Sull In**, Daegu Gyeongbuk Institute of Science and Technology, Republic of Korea

**Hiroshi Sakaguchi**, Kyoto University, Japan

**Xianjun Huang**, National University of Defence Technology, China

**Jaime Gomez Rivas**, Eindhoven University of Technology, The Netherlands  
**Jianguo Liu**, Nanjing University, China  
**Lingling Huang**, Beijing Institute of Technology Beijing, China  
**Jinsub Park**, Hanyang University, Republic of Korea  
**Xudong Zhao**, University of Hull, United Kingdom  
**Zhangxiong Wu**, Soochow University, China  
**Abul K Azad**, Los Alamos National Laboratories, USA  
**Peng Wang**, King Abdullah University of Science and Technology, Saudi Arabia  
**Seongil Im**, Yonsei University, Republic of Korea  
**Mukul Kabir**, Indian Institute of Science Education and Research, India  
**Yang Yan**, Dalian University of Technology, China  
**Yanzhong Zhang**, Donghua University, China  
**Zhifei Dai**, Peking University, China  
**Ioana Demetrescu**, Politehnica University of Bucharest, Romania  
**Jiashing Yu**, National Taiwan University, Taipei

## **Advisory Committee**

**Bharat Bhushan**, Ohio Eminent Scholar and The Howard D. Winbigler Professor, The Ohio State University, USA  
**Junhong Chen**, ASME Fellow, NAI Fellow, UWM Distinguished Professor, UW System Regent Scholar, University of Wisconsin-Milwaukee, USA  
**Dion Dionysios**, Fellow of the American Chemical Society, University of Cincinnati, USA  
**Alain Dufresne**, Top 300 most cited researchers in materials science and engineering, Grenoble INP Pagora, France  
**Hannu Häkkinen**, Member of the Finnish Academy of Science and Letters, University of Jyväskylä, Finland  
**Eric M.V. Hoek**, Professor & Industrial Affiliates Program Director Environmental Engineering, University of California Los Angeles, USA  
**Zhiqiang Hu**, Department Chair Civil and Environmental Engineering, University of Missouri, USA  
**Bin Liu**, Provost's Chair professor, National University of Singapore, Singapore  
**Kostya Ostrikov**, Pawsey Medal citation of the Australian Academy of Sciences, Queensland University of Technology, Australia  
**Yugang Sun**, Over 220 publications (H index 70), Temple University, USA  
**Ziqi Sun**, ARC DECRA Fellow, Queensland University of Technology, Australia  
**Ben Zhong Tang**, Member of Chinese Academy of Sciences, The Hong Kong University of Science & Technology, Hong Kong SAR  
**Thomas J. Webster**, The Art Zafiropoulo Chair and Professor, Northeastern University, USA  
**Guobao Xu**, Fellow and Chartered Scientist of Royal Society of Chemistry, University of Chinese Academy of Science, China  
**Yuegang Zhang**, National "Thousand Talents Program " Specially Recruited Expert, Tsinghua University, China  
**Chunyi Zhi**, Over 265 publications (H index 60), City University of Hong Kong, Hong Kong SAR

## **Scientific Program Committee**

**Sandeep Kumar**, Soft Condensed Matter Group, Raman Research Institute, India

**Jinglong Gong**, Tianjin University, China  
**Hao Jiang**, East China University of Science and Technology, China  
**Zhe Liu**, Wenzhou Institute of Biomaterials and Engineering, CAS, China  
**CJ Luo**, University College London, United Kingdom  
**Shlomo Magdassi**, The Hebrew University of Jerusalem, Israel  
**Xianqiang Mi**, Shanghai Advanced Research Institute, CAS, China  
**C.N.R. Rao**, Jawaharlal Nehru Centre for Advanced Scientific Research, India  
**Jianping Xie**, National University of Singapore, Singapore  
**Ying-Wei Yang**, Jilin University, China  
**Mo Yang**, The Hong Kong Polytechnic University, Hong Kong SAR  
**Zhi Yang**, Shanghai Jiao Tong University, China

## **Organizing Committee**

**Giovanni Benelli**, University of Pisa, Italy  
**Wei Guo**, Technical Institute of Physics and Chemistry, CAS, China  
**Munawar Khalil**, University of Indonesia, Indonesia  
**Zhanfang Ma**, Capital Normal University, China  
**Jayakumar Rangasamy**, Amrita Institute of Medical Sciences and Research Centre, India  
**Uma Shanker**, Dr B R Ambedkar National Institute of Technology Jalandhar, India  
**Wei Wu**, Wuhan University, China  
**Chi Yang**, National University of Singapore, Singapore  
**Xin Wu**, Colorado School of Mines, USA  
**Zhihua Zhou**, Shanghai Jiao Tong University, China

Sponsored By



SHANGHAI JIAO TONG  
UNIVERSITY



Nano-Micro  
Letters



Key Laboratory for Thin Film and Microfabrication  
of Ministry of Education

Shanghai Jiao Tong University

Nano-Micro Letters, a Springer Open Access Journal, No Publication Fee, 2017 IF 7.381

Key Laboratory for Thin Film and Microfabrication of Ministry of Education, China



Nature Research Society

120 Baker Street, Westminster, W1U 6TU, London, United Kingdom



The Department of Chemistry,  
Sungkyunkwan Univ.



## Registration desk hours

The Nano-Micro Conference 2018 registration desk, located outside the meeting rooms, will be open during the following hours:

Data	Time
Sunday, December 16 <sup>th</sup>	2:00pm – 6:00pm
Monday, December 17 <sup>th</sup>	8:30am – 6:00pm
Tuesday, December 18 <sup>th</sup>	8:30am – 6:00pm
Wednesday, December 19 <sup>th</sup>	8:30am – 6:00pm

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

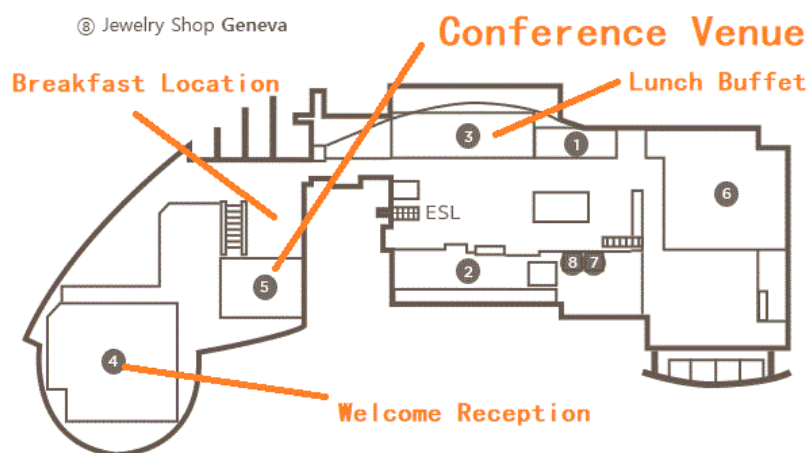
**Location:** Ramada Plaza Jeju ([Ramada Plaza by Wyndham Jeju Ocean Front](#))

**Address:** 66 Tapdong ro Jeju-si, Republic Of Korea +82-64-7298224

**Meeting Room:** The Second floor, MEETING Room A, Room B, Room C

### Floor Information 2F

- ① Lobby Lounge Scotra
- ② Front
- ③ Western & Buffet Restaurant The Blue
- ④ Banquet Ramada Ballroom
- ⑤ Semina Room
- ⑥ Casino
- ⑦ Business Center
- ⑧ Jewelry Shop Geneva



<p><b>Nano-Micro Conference 2018</b></p> <p>December 17th – December 20th</p> <p>Ramada Plaza Jeju, Jeju-si, Jeju Island, Republic of Korea</p>
<p><b>Sunday, December 16 2018</b></p> <p>14:00 – 18:00</p> <p>Conference On-site Registration</p> <p>Location: Ramada Plaza Jeju</p> <p><a href="#">(Ramada Plaza by Wyndham Jeju Ocean Front)</a></p>

<p><b>Monday, December 17 2018</b></p> <p>Room A</p>		
8:00-9:00AM	Coffee Breakfast (Location: Near the conference registration desk)	
<p><b>Keynote Talk</b></p> <p><b>Chair: Saskia F. Fischer</b></p>		
9:00-9:45AM	K01: Topological Phases of Quantum Matter, Novel Superconductors, and Ultra-Thin Films Beyond Graphene	<p><b>Arun Bansil</b></p> <p>Northeastern University, USA</p>
9:45-10:30AM	K02: Graphene: The Thinnest Known Coating for Corrosion Protection	<p><b>Raman Singh</b></p> <p>Monash University, Australia</p>
10:30-11:00AM	<b>Coffee Break</b>	
<p><b>December 17 2018, Room A</b></p> <p><b>Monday</b></p> <p><b>Session A1: Topological Insulators</b></p> <p><b>Chair: Arun Bansil</b></p>		
11:00-11:30AM	A01: Photovoltaic anomalous Hall effect and orbital effect in line-node semimetals	<p><b>Katsuhisa Taguchi</b></p> <p>Kyoto University, Japan</p>
11:30-12:00PM	A02: Topological Surface States and Two-Dimensional Layered Transport in bulk $\text{Bi}_2\text{Se}_3$	<p><b>Saskia F. Fischer</b></p> <p>Humboldt-Universität zu Berlin, Germany</p>
12:00-14:00PM	<b>Lunch Break</b> (Buffet, <a href="#">The Blue Restaurant</a> )	



<p style="text-align: center;"><b>December 17 2018, Room A</b>  <b>Monday</b>  <b>Session A2: Topological Insulators</b>  <b>Chair: Katsuhisa Taguchi</b></p>		
14:00-14:30PM	A03: Imaging stacking domain walls and topological edge states in bi- and trilayer graphene by STM/STS	<b>Long-Jing Yin</b> Hunan University, China
14:30-15:00PM	A04: Nuclear magnetic resonance in topological insulators: Bi <sub>2</sub> Te <sub>3</sub> and Bi <sub>2</sub> Se <sub>3</sub>	<b>Anastasia Antonenko</b> Saint Petersburg State University, Russia
15:00-15:30PM	A05: Graphene Supported Graphene/Graphene Bilayer Nanostructure Material for Spintronics	<b>Sekhar Chandra Ray</b> University of South Africa (UNISA), South Africa
15:30-16:00PM	<b>Coffee Break</b>	
<p style="text-align: center;"><b>December 17 2018, Room A</b>  <b>Monday</b>  <b>Session A3: Graphene and carbon nanomaterials</b>  <b>Chair: Sang-Yong Ju</b></p>		
16:00-16:30PM	A06: Large positive magnetoresistance in twisted few layer graphene	<b>Oleg Kononenko</b> Institute of Microelectronics Technology and High Purity Materials Russian Academy of Sciences, Russia
16:30-17:00PM	A07: Graphene nanotubes reinforced aluminum based superprofile	<b>Hansang Kwon</b> Pukyong National University, Republic of Korea
17:00-17:30PM	A08: Electron emission theories for 2D-materials and applications	<b>Ricky Lay-Kee Ang</b> Singapore University of Technology and Design, Singapore
17:30-18:00PM	A09: Graphene nanoribbons formed by a sonochemical graphene unzipping using supramolecular template	<b>Sang-Yong Ju</b> Yonsei University, Republic of Korea
19:00-21:00PM	<b>Welcome Reception</b>	

Monday, December 17 2018 Room B		
8:00-9:00AM	Coffee Breakfast (Location: Near the conference registration desk)	
<b>Keynote Talk</b> <b>Chair: Ray Chen</b>		
9:00-9:45AM	K03: Synthesis of Two Different Types of Phase-selectively Disordered Blue TiO <sub>2</sub> Nanomaterials and their Applications	<b>Hyoyoung Lee</b> Sungkyunkwan University, Republic of Korea
9:45-10:30AM	K04: Highly Efficient Photoconversion of CO <sub>2</sub> : Controllable Transition from C1 to C2 Products	<b>Su-il In</b> Daegu Gyeongbuk Institute of Science and Technology, Republic of Korea
10:30-11:00AM	Coffee Break	
<b>December 17 2018, Room B</b> <b>Monday</b> <b>Session B1: Nanomaterials for Energy and Environmental Applications</b> <b>Chair: Elijah Thimsen</b>		
11:00-11:30AM	B01: Effective solar energy conversion based on spectral control of thermal radiation via monolithic absorber/emitter	<b>Makoto Shimizu</b> Tohoku University, Japan
11:30-12:00PM	B02: MoS <sub>2</sub> -based electrocatalysts for hydrogen evolution catalysis: a comparative study on synthesis methods	<b>Yo-Sep Min</b> Konkuk University, Republic of Korea
12:00-12:30PM	B03: Novel concept of intermediate band for III-V Nitride solar cells	<b>Liwen Sang</b> National Institute for Materials Science (NIMS), Japan

12:30-14:00PM	<b>Lunch Break</b> (Buffet, <a href="#">The Blue Restaurant</a> )	
<b>December 17 2018, Room B</b> <b>Monday</b> <b>Session B2: Nanomaterials for Energy and Environmental Applications</b> <b>Chair: Liwen Sang</b>		
14:00-14:30PM	B04: A high throughput synthesis of semiconductor nanocrystals and preparation of highly luminescent composite beads for LEDs	<b>Young-Kuk Kim</b> Korea Institute of Materials Science (KIMS), Republic of Korea
14:30-15:00PM	B05: Two-dimensional semiconductor based transparent solar cell and its performance enhancement	<b>Ah-Jin Cho</b> Yonsei University, Republic of Korea
15:00-15:30PM	B06: Modulation by modelling of the morphology of (nano) micromaterials	<b>Amanda Fernandes Gouveia</b> Federal University of São Carlos, Brazil
15:30-16:00PM	Coffee Break	
<b>December 17 2018, Room B</b> <b>Monday</b> <b>Session B3: Nanomaterials for Energy and Environmental Applications</b> <b>Chair: Sull In</b>		
16:00-16:30PM	B08: Magnetically recyclable Z-scheme photocatalyst for organic pollutants removal in aqueous media	<b>Lu Gan</b> Nanjing Forestry University, China
16:30-17:00PM	B09: Electron transport characteristics of films comprised of transparent conducting nanocrystals synthesized by plasma	<b>Elijah Thimsen</b> Washington University in St. Louis, USA
17:00-17:30PM	B10: Noble photocatalytic systems for degradation and detection of pollutants towards wastewater treatment applications	<b>Raju Kumar Gupta</b> Indian Institute of Technology Kanpur, India
19:00-21:00PM	<b>Welcome Reception</b>	

Tuesday, December 18 2018 Room A		
8:00-9:00AM	Coffee Breakfast (Location: Near the conference registration desk)	
<b>Session A4: Graphene and carbon nanomaterials</b> <b>Chair: Hiroshi Sakaguchi</b>		
9:00-9:30AM	A10: Nanoporous gold for sensor and fuel cell catalysts	<b>Jianguo Liu</b> Nanjing University, China
9:30-10:00AM	A11: Sensitive Room-Temperature H <sub>2</sub> S Gas Sensors Employing SnO <sub>2</sub> Quantum Wire/Reduced Graphene Oxide Nanocomposites	<b>Huan Liu</b> Huazhong University of Science and Technology, China
10:00-10:30AM	A12: Screened strong light-matter coupling of excitons in multilayer 2D-semiconductors and plasmonic nanocavities	<b>Jaime Gomez Rivas</b> Eindhoven University of Technology (TU/e), The Netherlands
10:30-11:00AM	Coffee Break	
<b>December 18 2018, Room A</b> <b>Tuesday</b> <b>Session A5: Graphene and carbon nanomaterials</b> <b>Chair: Xianjun Huang</b>		
11:00-11:30AM	A13: Functional Molecular Junctions derived from Double Self-assembled Monolayers on Graphene	<b>Sohyeon Seo</b> Sungkyunkwan University, Republic of Korea
11:30-12:00PM	A14: Spin-valley transport property in silicene junction	<b>Bunned Soodchomshom</b> Kasetsart University, Thailand
12:00-12:30PM	A15: Comparison of electrical energy and power of PV cells or module with different cells materials in clear sky day condition	<b>Rohit Tripathi</b> Galgotias University, India

12:30-14:00PM	<b>Lunch Break</b> (Buffet, <a href="#">The Blue Restaurant</a> )	
<b>December 18 2018, Room A</b> <b>Tuesday</b> <b>Session A6: Graphene and carbon nanomaterials</b> <b>Chair: Jaime Gomez Rivas</b>		
14:00-14:30PM	A16: Printed graphene nanoflakes for radio frequency antennas and wireless sensors	<b>Xianjun Huang</b> National University of Defence Technology, China
14:30-15:00PM	A17: Bio-inspired on-surface fabrication of graphene nanoribbons	<b>Hiroshi Sakaguchi</b> Kyoto University, Japan
15:00-15:30PM	A18: Facile Synthesis of 2D Nitrogen-Containing Porous Carbon Nanosheets Induced by Graphene Oxide for High-Performance Supercapacitors	<b>Xu Zhang</b> Dalian University of Technology, China
15:30-16:00PM	Coffee Break	
<b>December 18 2018, Room A</b> <b>Tuesday</b> <b>Session A7: Graphene and carbon nanomaterials</b> <b>Chair: Jianguo Liu</b>		
16:00-16:30PM	A19: Electrochemical Synthesis of Nano-Structured Si for Energy Storage Application	<b>Indrajit Mukhopadhyay</b> Pandit Deendayal Petroleum University, India
16:30-17:00PM	A20: Coherent phonons of high- and low-symmetry in the topological insulators	<b>Oleg Misochko</b> Institute of Solid State Physics, Russian Academy of Sciences, Russia
17:00-17:30PM	A21: Switchable valley polarization by external electric field effect in graphene/CrI <sub>3</sub> heterostructures	<b>Jisang Hong</b> Pukyong National University, Republic of Korea

<p>Tuesday, December 18 2018 Room B</p>		
8:00-9:00AM	Coffee Breakfast (Location: Near the conference registration desk)	
<p><b>Session B4</b>  <b>Nanomaterials for Energy and Environmental Applications</b>  <b>Chair: Lingling Huang</b></p>		
9:00-9:30AM	B11: Metasurfaces for Solar Thermophotovoltaic Energy Harvesting	<p><b>Abul K. Azad</b>  Los Alamos National Laboratories,  USA</p>
9:30-10:00AM	B12: Solar cell and photoelectrochemical properties of Cu <sub>2</sub> ZnSnS <sub>4</sub> thin films fabricated by wet chemical techniques	<p><b>Shigeru Ikeda</b>  Konan University, Japan</p>
10:00-10:30AM	B13: A novel absorber material ZnSnP <sub>2</sub> - crystal growth and device	<p><b>Yoshitaro Nose</b>  Kyoto University, Japan</p>
10:30-11:00AM	Coffee Break	
<p><b>December 18 2018, Room B</b>  <b>Tuesday</b>  <b>Session B5: Nanomaterials for Energy and Environmental Applications</b>  <b>Chair: Jinsub Park</b></p>		
11:00-11:30AM	B14: Solar energy conversion to high-value-added reagents on nanoporous sponge photoanodes	<p><b>Tomohiko NAKAJIMA</b>  National Institute of Advanced Industrial Science and Technology,  Japan</p>
11:30-12:00PM	B15: Key technologies for the novel solar driven heating and cooling systems	<p><b>Xudong Zhao</b>  University of Hull, United Kingdom</p>

12:00-14:00PM	<b>Lunch Break</b> (Buffet, <a href="#">The Blue Restaurant</a> )	
<b>December 18 2018, Room B</b> <b>Tuesday</b> <b>Session B6: Nanophotonic Devices and Materials</b> <b>Chair: Xudong Zhao</b>		
14:00-14:30PM	B16: Silicon Photonics for 2020 and beyond	<b>Ray Chen</b> The University of Texas, USA
14:30-15:00PM	B17: Light emission effects mediated by Bloch Surface Waves	<b>Emiliano Descrovi</b> Politecnico di Torino, Italy
15:00-15:30PM	B18: High-dimensional vectorial holographic encryption with metasurfaces	<b>Lingling Huang</b> Beijing Institute of Technology Beijing, China
15:30-16:00PM	Coffee Break	
<b>December 18 2018, Room B</b> <b>Tuesday</b> <b>Session B7: Nanophotonic Devices and Materials</b> <b>Chair: Abul K Azad</b>		
16:00-16:30PM	B19: Application of transferable ZTO nanosphere monolayers to optoelectronic devices	<b>Jinsub Park</b> Hanyang University, Republic of Korea
16:30-17:00PM	B20: Development and characterization of metallo-dielectric nanomaterials	<b>Yan Hong</b> University of Electronic Science and Technology of China, China
17:00-17:30PM	B21: Electrons dynamics control in ultrafast laser micro/nanofabrication by spatially/temporally shaped pulses	<b>Xiaowei Li</b> Beijing Institute of Technology Beijing, China
17:30-18:00PM	B22: Plasmon-enhanced nanoscopy for nanoscale analysis	<b>Taka-aki Yano</b> Tokyo Institute of Technology, Japan

Room C Tuesday, December 18 2018 Poster Session		
8:00-9:00AM	Coffee Breakfast (Location: Near the conference registration desk)	
<b>10:30-11:00; 15:30-16:00;</b>		
P1	Dimension-dependent Perovskite-metal oxide core-shell nanocrystals for CO <sub>2</sub> reduction	<b>Yunhee Cho</b> Sungkyunkwan University, Republic of Korea
P2	Continuous degradation of toxic molecules through in-situ reduction of CO <sub>2</sub> using metal doped B-TiO <sub>2</sub> photocatalysts	<b>Hee Min Hwang</b> Sungkyunkwan University, Republic of Korea
P3	Ultraviolet photodetector using pn junction of p-CuO hollow nanospheres and n-ZnO nanorods	<b>Yuexing Ji</b> Hanyang University, Republic of Korea
P4	Highly carbon-doped TiO <sub>2</sub> derived from MXene boosting the photocatalytic hydrogen evolution	<b>Guangri Jia</b> Jilin University, China
P5	Hexagonal FeIn <sub>2</sub> S <sub>4</sub> : Layer Dependent Band Structure of Ternary Metal Chalcogenides	<b>Hyunjung Kim</b> Sungkyunkwan University, Republic of Korea
P6	Ligand exchanged colloidal WSe <sub>2</sub> and its counter cation dependent HER study	<b>Meeree Kim</b> Sungkyunkwan University, Republic of Korea
P7	The Fabrication of ZnO Nanoarrays and Its Applications for Photoelectrochemical Water Splitting and Protein Microarray based Biosensing	<b>Chang Liu</b> Jilin University, China
P8	Electrochemical fabrication of hierarchical pseudocapacitive electrode for supercapacitor	<b>Xiaoxia Liu</b> Northeastern University, China



P9	Energy Band Modulation of Phase-selectively Disordered Pt-TiO <sub>2</sub> for Highly Active Photocatalysts	<b>Simgeon Oh</b> Sungkyunkwan University, Republic of Korea
P10	The effects of Ga <sub>2</sub> O <sub>3</sub> interlayer on the emission of n-In <sub>2</sub> O <sub>3</sub> nanorod/p-GaN heterojunction light emitting diode	<b>Dong Su Shin</b> Hanyang University, Republic of Korea
P11	Silver-incorporated Cu <sub>2</sub> ZnSnS <sub>4</sub> thin film as an absorber for solar cells and a cathode for photoelectrochemical water splitting	<b>Takato Kawaguchi</b> Konan University, Japan
P12	Impacts of Zr-doping into crystalline lattices of bismuth vanadate powder and thin film on their photocatalytic and photoelectrochemical properties	<b>Takato Kawaguchi</b> Konan University, Japan
P13	Graphene quantum dots decorated graphene as an enhanced sensing platform for sensitive and selective detection of copper(II)	<b>Ying Wang</b> Jilin University, China
P14	Elastic nanoscale spongy graphene-functionalized silicon as excellent stability anode in Li ion battery	<b>Jong-Sung Yu</b> Daegu Gyeongbuk Institute of Science and Technology, Republic of Korea
P15	Structure and visible-light induced photocatalytic activity of metal cyanamide composites	<b>Xia Zhang</b> Department of Chemistry, Northeastern University, China
P16	Nanoporous Sulfur-doped Copper Oxide (Cu <sub>2</sub> O <sub>x</sub> S <sub>1-x</sub> ) for Overall Water Splitting	<b>Xiaolin Zhang</b> Jilin University, China

Wednesday, December 19 2018 Room A		
8:00-9:00AM	Coffee Breakfast (Location: Near the conference registration desk)	
<b>Session A8: 2D Materials</b> <b>Chair: Peng Wang</b>		
9:00-9:30AM	A22: Multiscale Modeling of Heat Transfer in Low-Dimensional Materials	<b>Yuan Dong</b> University of Missouri, USA
9:30-10:00AM	A23: Advanced materials and processes for Silicon based solar cells	<b>Rosaria Puglisi</b> Institute for Microelectronics and Microsystems, Italy
10:00-10:30AM	A24: Vacancy diffusion in graphene	<b>Mukul Kabir</b> Indian Institute of Science Education and Research, India
10:30-11:00AM	Coffee Break	
<b>December 19 2018, Room A</b> <b>Wednesday</b> <b>Session A9: 2D materials</b> <b>Chair: Seongil Im</b>		
11:00-11:30AM	A25: Chirality Effects on an Electron Transport in Single-walled Carbon Nanotube	<b>Suthee Boonchui</b> Kasetsart University, Thailand
11:30-12:00PM	A26: Ionic liquids assisted synthesis of porous carbon materials for energy storage devices	<b>Yang Yan</b> Dalian University of Technology, China
12:00-14:00PM	<b>Lunch Break</b> (Buffet, <a href="#">The Blue Restaurant</a> )	

**December 19 2018, Room A**  
**Wednesday**  
**Session A10: Nanomaterials for Energy and Environmental Applications**  
**Chair: Mukul Kabir**

14:00-14:30PM	A28: Intrinsic field effect and Hall mobility in multilayer III-VI 2D semiconductor InSe FETs	<b>Sukrit Sucharitakul</b> RIKEN Center for Emergent Matter Science, Japan
14:30-15:00PM	A29: Nano-enabled clean water production by sunlight	<b>Peng Wang</b> King Abdullah University of Science and Technology, Saudi Arabia
15:00-15:30PM	A30: Thin Graphite Contact for 2D-Layered Material CMOS Device and Band Gap Estimation	<b>Seongil Im</b> Yonsei University, Republic of Korea
15:30-16:00PM	Coffee Break	

**December 19 2018, Room A**  
**Wednesday**  
**Session A11: 2D Materials**  
**Chair: Yang Yan**

16:00-16:30PM	A31: Energy dissipation and light emission in graphene	<b>Myung-Ho Bae</b> Korea Research Institute of Standards and Science, Republic of Korea
16:30-17:00PM	A32: Unexpectedly Promoting Effect of Carbon Nanotubes Grown During the Non-oxidative Coupling of Methane over Copper Catalysts	<b>Jarrn-Horng Lin</b> National University of Tainan, Tainan

Wednesday, December 19 2018 Room B		
8:00-9:00AM	Coffee Breakfast (Location: Near the conference registration desk)	
<b>Session B8: Nanomaterials for Biomedical Applications</b> <b>Chair: Yanzhong Zhang</b>		
9:00-9:30AM	B23: Micro and nanocoatings for biomedical applications improving Ti50Zr alloy performance	<b>Ioana Demetrescu</b> Politehnica University of Bucharest, Romania
9:30-10:00AM	B24: Plasmonic semiconductors for photothermal therapy in the NIR-II window	<b>Jiang Jiang</b> International Lab of Adaptive Biotechnology, SINANO, CAS, China
10:00-10:30AM	B25: Janus Drug-Drug Conjugate Nanocapsules for enhancing Cancer Therapeutic Efficacy	<b>Zhifei Dai</b> Peking University, China
10:30-11:00AM	Coffee Break	
<b>December 19 2018, Room B</b> <b>Wednesday</b> <b>Session B9: Nanomaterials for Biomedical Applications</b> <b>Chair: Zhifei Dai</b>		
11:00-11:30AM	B26: Formation of micro/nano wrinkles on polymeric surfaces	<b>Dae Kun Hwang</b> Ryerson University, Canada
11:30-12:00PM	B27: A Novel "Micro-capillary ELISA" for Detecting Salivary Biomarkers Aiming for POC Applications	<b>Young Jun Kim</b> Electronics & Telecommunications Research Institute, Republic of Korea
12:00-12:30PM	B28: Surface Modification of ZnO Nanoparticles by Core-Shell Nanoparticles Decreased Cytotoxicity towards HeLa Cancer Cells: A facile Approach for Safer Nanomaterials	<b>Amna Sirelkhatim</b> Sudan University of Science and Technology, Sudan

12:30-14:00PM	<b>Lunch Break</b> (Buffet, <a href="#">The Blue Restaurant</a> )	
<b>December 19 2018, Room B</b> <b>Wednesday</b> <b>Session B10: Nanomaterials for Biomedical Applications</b> <b>Chair: Ioana Demetrescu</b>		
14:00-14:30PM	B29: Shape memory fibrous scaffolds for bone tissue engineering	<b>Yanzhong Zhang</b> Donghua University, China
14:30-15:00PM	B30: Capped gold and silver clusters as efficient contrast agents for bio-imaging? Exploring new routes to enhance their emission properties	<b>Rodolphe Antoine</b> CNRS et Université Lyon 1, France
15:00-15:30PM	B31: Peptide-Modified PLL-coated Aligned PEDOT:PSS Fibers Promotes the Growth of PC12-derived Nerve Cells	<b>Jiashing Yu</b> National Taiwan University, Taipei
15:30-16:00PM	Coffee Break	
<b>December 19 2018, Room B</b> <b>Wednesday</b> <b>Session B11: Nanomaterials for Biomedical Applications</b> <b>Chair: Jiashing Yu</b>		
16:00-16:30PM	B32: Bio-Hybrid Hydrogel Comprising Animal and Plant Sources Embedded with Protein Capped Silver Nanoparticles for Accelerated Tissue Regeneration in Chronic Tissue Defects	<b>Palanisamy Thanikaivelan</b> CSIR-Central Leather Research Institute Adyar, India
16:30-17:00PM	B33: Multifunctional Bio-Plasmonic and Luminescent Nanomaterials for Smart Biosensors and Theranostics Applications	<b>Yen Nee TAN</b> Newcastle University (Singapore Campus), Singapore
17:00-17:30PM	B34: T1/T2 Dual functional iron oxide MRI contrast agent with super stability and low hypersensitivity	<b>Hongchen Gu</b> Shanghai Jiao Tong University, China
17:30-18:00PM	B35: Nanotechnology and Environmental Application: Future with Electrospinning	<b>Shivendu Ranjan</b> University of Johannesburg, South Africa

**Thursday, December 20 2018**

All Day Tour, 9:00 - 6:00PM

**(Transportation, tickets & lunch covered)**

Meeting Point: Hotel Lobby (Second Floor)

Meeting Time: 9:00 AM

**Keynote Talk**

**9:00 - 9:45 AM Room A December 17**

# **K01: Topological Phases of Quantum Matter, Novel Superconductors, and Ultra-Thin Films Beyond Graphene**

Arun Bansil\*

*Northeastern University, Boston, Massachusetts, USA*

\*Corresponding author. Email: ar.bansil@northeastern.edu

## **Abstract**

I will discuss some of our recent work aimed at understanding the electronic structure and spectroscopy of novel superconductors, topological materials, and atomically thin 2D films beyond graphene. [1-6] Illustrative examples will include: (i) How by exploiting electronic structure techniques we have been able to successfully predict and understand the characteristics of many new classes of binary, ternary and quaternary topologically interesting materials, including topological crystalline insulators and Weyl and other more exotic semi-metallic topological phases; (ii) How atomically thin ‘beyond graphene’ 2D and layered materials offer exciting new possibilities for manipulating electronic structures and provide novel platforms for fundamental science and applications; (iii) With regard to the high-T<sub>c</sub>’s, I will discuss recent breakthroughs in modeling first-principles the insulating pristine compounds and the transition from the insulating to the metallic state with doping without invoking any free parameters such as U. A first-principles description of the competing stripe and magnetic phases in the cuprates also then becomes possible, providing a new pathway for modeling correlated materials more generally.

## **References**

- [1] Bansil, Lin and Das, *Reviews of Modern Physics* 88, 021004 (2016)
- [2] Xu et al., *Science Advances* 3, e1603266 (2017)
- [3] Vargas et al., *Science Advances* 3, e1601741 (2017)
- [4] Hafiz et al., *Science Advances* 3, e1700971 (2017)
- [5] Furness et al., *Nature Communications Physics* 1, 11 (2018)
- [6] C. Lane et al., *Physical Review B* 98, 125140 (2018)

***Keynote Talk***

***9:45 - 10:30 AM Room A December 17***

**K02: Graphene: The Thinnest Known Coating for Corrosion Protection**

Raman Singh\*

*Monash University, Australia*

\*Corresponding author. Email: raman.singh@monash.edu

**Abstract**

Graphene, a two-dimensional (2-D) atomically thin film of carbon atoms, has unique characteristics that have triggered unprecedented research excitement. Besides several other unique properties, graphene possesses remarkable chemical inertness. Graphene coatings either a single or a few atomic layers thick on metals has been shown to improve their corrosion resistance by up to one-and-half orders of magnitude. Although the studies on this topic are limited to just a few carried out in 2011–2013, great variability is found in the extent of corrosion resistance from graphene reported in these studies. This article presents a brief review of graphene as a corrosion-protecting coating, identifies potential and presents some new data to suggest graphene as durable corrosion-resistant coating.

***Keywords***

Corrosion Resistance; Electrochemical Impedance Spectroscopy; Duplex Stainless Steel; Graphene Film; Chemical Vapor Deposition Process



**Session A1**

**11:00 - 11:30 AM Room A December 17**

**A01: Photovoltaic anomalous Hall effect and orbital effect in line-node semimetals**

Katsuhisa Taguchi\*

*Yukawa Institute Theoretical Physics, Kyoto University, Kitashirakawa Oiwakecho, Sakyo-ku  
Kyoto 606-8502, Japan*

\*Corresponding author. Email: katsuhisa.taguchi@yukawa.kyoto-u.ac.jp

**Abstract**

To show characteristic phenomena in line-node semimetal, which is one of the topological materials generated by a closed loop shape touching between multiple valance and conduction bands, we theoretically study photovoltaic anomalous Hall effect as well as the orbital magnetization in line-node semimetal in the presence of a circularly polarized light. When the polarized light propagates along the direction to break mirror-symmetry of the close loop of the multiple band touching, unconventional photovoltaic interaction is emerged, and nonzero Berry curvature is generated. This work discusses the light frequency and electric fields of light dependency of the photovoltaic interaction. In the presence of the photovoltaic interaction, there is nonzero Berry curvature, and the orbital magnetization is generated. Besides, anomalous Hall current is triggered when we additionally apply an external electric field perpendicular to the surface of the closed loop. These phenomena could be applicable for optical devices.

**Keywords**

Photovoltaic anomalous Hall effect; Line-node semimetal

**Introduction**

Recently, topological materials with linear energy dispersion in multiple bands, which host Dirac fermions and Weyl fermions, have been studied in condensed matter physics. For example, in three-dimensional topological insulators, there are Dirac fermions on the surface of topological insulators, where the Dirac fermions have unconventional spin-momentum locking because of strong spin-orbit coupling. As a result, unconventional characteristic charge transports have been revealed. These characteristic phenomena are caused by nonzero Berry curvature at the point node of the multiple bands. On the other hand, it is possible to make a closed line node by touching between multiple conduction band and valance bands. The materials are named as line-node semimetals. The dimension of nodes of the line-node semimetal is different from that of a point node, and unconventional transport via the nodes have been expected. In this work, to show characteristic phenomena in line-node semimetals, we consider the photovoltaic anomalous Hall effect as well as orbital magnetization in a line-node semimetal.

**Methods**

The photovoltaic anomalous Hall effect is calculated by using Green's function techniques in an effective model Hamiltonian of the line-node semimetal with an applied circularly polarized light. The photovoltaic anomalous Hall effect is generated by nonzero the photovoltaic interaction. Its interaction is given by the effective Hamiltonian of the line-node semimetal with and without applied circularly polarized light shown in Reference [1]. The effective Hamiltonian with circularly polarized light is obtained by using the Floquet method within the second harmonic electric fields of the polarized light. The detail procedure is shown in literature [2].

## Results and Discussion

From the above method, the photovoltaic interaction indicates the coupling between spin angular momentum of the circularly polarized light and momentum of electrons. The coefficient of its interaction  $L_y$  is proportional to the square of the electric field  $E$  of the polarized light as shown in Figure 1(a). In addition, the chemical potential of the line-node semimetal  $\mu$  is also changed by  $\delta\mu$ . [Figure 1(b)].

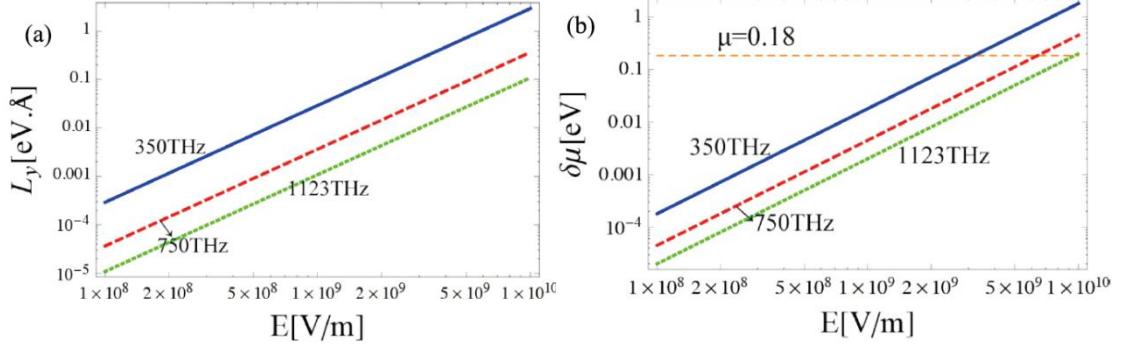


Figure 1. The electric field  $E$  dependence of (a) the coefficient of photovoltaic interaction  $L_y$  and (b) the photovoltaic chemical potential  $\delta\mu$  for several frequency of the polarized light. These figures are based on realistic parameters, which are the same as those used in Fig.2 in Reference [2].

In the presence of photovoltaic interaction, it is found that nonzero Berry curvature is generated. In generally, the Berry curvature relates the orbital magnetization [3]. From its analogy, nonzero orbital magnetization could be emerged only when the circularly polarized light is traveling along the mirror-symmetry breaking direction. It could be evidence for the characteristic phenomena of line-node semimetal without using an external applied electric field, if the orbital magnetization could be measured.

## Conclusions

We theoretically study the light-induced anomalous Hall current and orbital magnetization in line-node semimetals. It is found that in the presence of the circularly polarized light, nonzero Berry curvature is generated by the photovoltaic interaction between spin angular momentum of light and momentum of electrons. As a result, the orbital magnetization and the photovoltaic anomalous Hall effect are triggered. They could be applicable to optical devices based on the anisotropic optical properties of line-node semimetals.

## Acknowledgement

This work was supported by YITP of Kyoto University.

## References

- [1] Y. Kim, B. J. Wieder, C. L. Kane, and A. M. Rappe, Phys. Rev. Lett. 115, 036806 (2015). doi: 10.1103/PhysRevLett.115.036806
- [2] K. Taguchi, D.-H. Xu, A. Yamakage, and K. T. Law, Phys. Rev. B 94, 155206 (2016). doi: 10.1103/PhysRevB.94.155206
- [3] W. Yao, D. Xiao, and Q. Niu, Phys. Rev. B 77, 235406 (2008). doi: 10.1103/PhysRevB.77.235406

**Session A1**

**11:30 - 12:00 PM Room A December 17**

**A02: Topological Surface States and Two-Dimensional Layered Transport  
in bulk Bi<sub>2</sub>Se<sub>3</sub>**

O. Chiatti<sup>1</sup>, M. Busch<sup>1</sup>, S. Pezzini<sup>2</sup>, S. Wiedmann<sup>2</sup>, O. Rader<sup>3</sup>, L.V. Yashina<sup>4</sup>, S. F. Fischer<sup>1,\*</sup>

<sup>1</sup>*Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany*

<sup>2</sup>*High Field Magnet Laboratory, Radboud University Nijmegen, 6525ED Nijmegen, The Netherlands*

<sup>3</sup>*Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany*

<sup>4</sup>*Department of Chemistry, Moscow State University, 119991 Moscow, Russia*

\*Corresponding author. Email: sfischer@physik.hu-berlin.de

**Abstract**

Helically spin-polarized Dirac fermions in topologically protected surface states are of high interest as a new state of quantum matter and they are studied in so-called topological insulators (TI). However, we found that in a prototypical three-dimensional TI material, Bi<sub>2</sub>Se<sub>3</sub>, the magneto-transport experiments indicate that these surface states may coexist with a layered two-dimensional electron system in the bulk [1]. Recently, we demonstrated quantization effects in the Hall resistance at temperatures up to 50 K in nominally undoped bulk Bi<sub>2</sub>Se<sub>3</sub> single crystals with a high electron density ( $n \sim 2 \cdot 10^{19} \text{ cm}^{-3}$ ). From the angular and temperature dependence of the Hall resistance and the Shubnikov-de Haas oscillations we identify 3D and 2D contributions to transport. Angular resolved photoemission spectroscopy proves the existence of TSS. Here, I will outline a model for Bi<sub>2</sub>Se<sub>3</sub> and suggest that the coexistence of TSS and 2D layered transport may stabilize the quantum oscillations of the Hall resistance [2].

**Keywords**

Topological Surface States; Two-Dimensional Layered Transport; Magneto-transport; Quantum oscillations; Bi<sub>2</sub>Se<sub>3</sub> single crystals

**References**

- [1] O. Chiatti et al., Scientific Reports 6, 27483 (2016)
- [2] M. Busch et al., Scientific Reports 8, 485 (2018)

**Session A2**

**14:00 - 14:30 PM Room A December 17**

**A03: Imaging stacking domain walls and topological edge states in bi- and tri-layer graphene by STM/STS**

Long-Jing Yin<sup>1,2,\*</sup>, Lin He<sup>2</sup>

<sup>1</sup>*School of Physics and Electronics, Hunan University, Changsha, China*

<sup>2</sup>*Center for Advanced Quantum Studies, Department of Physics, Beijing Normal University, Beijing, China*

\*Corresponding author. Email: yinlj@hnu.edu.cn

**Abstract**

Looking for systems where topological edge states persist in the absence of external magnetic fields boosts rapid developments in condensed matter physics in the past few years. Gapped graphene bilayer with smooth domain walls is predicted to be one of the most promising candidates where charge carriers can travel long distances without dissipation. Although it has been extensively studied in theory, a direct imaging of topological edge states in bilayer graphene domain walls is still missing. The experimental challenge comes from both the fabrication of bilayer graphene sample which contains AB-BA domain wall and the precise measurement of the topological edge states at such stacking boundary. Here, we present direct imaging of the topologically protected 1D conducting channels in the AB-BA domain wall in exfoliated graphene bilayer [1]. With the help of the high-resolution scanning tunnelling microscope (STM) [2-5], we successfully detected the AB-BA domain wall structure in exfoliated graphene bilayer. Subsequently, we obtained the spatial distribution of the topological states around the domain wall for the first time via using the scanning tunnelling spectroscopy (STS) with high energy- and spatial-resolution. We found that the conducting edge states are mainly located at the two edges of the AB-BA domain wall and these states are quite robust even in the highest magnetic field  $\sim 8$  T of our STM system. The related experimental results are reproduced quite well by theoretical calculations. Moreover, we also imaged ABA-ABC trilayer graphene domain walls by using the same measurement technique [6]. Our studies directly confirm the existence of the topological edge states at AB-BA bilayer graphene domain wall, opening a wide vista of graphene-based topological transport properties.

**Keywords**

Topological edge states; graphene; domain wall; scanning tunnelling microscope (STM); scanning tunnelling spectroscopy (STS)

**References**

- [1] L.-J. Yin; H. Jiang; J.-B. Qiao; L. He, Direct imaging of topological edge states at a bilayer graphene domain wall. *Nature Communications*. 7, 11760 (2016). doi:10.1038/ncomms11760
- [2] L.-J. Yin; Y. Zhang; J.-B. Qiao; S.-Y. Li; L. He, Experimental observation of surface states and Landau levels bending in bilayer graphene. *Physical Review B*. 93, 125422 (2016). doi:10.1103/PhysRevB.93.125422
- [3] L.-J. Yin; J.-B. Qiao; W.-J. Zuo; W.-T. Li; L. He, Experimental evidence for non-Abelian gauge potentials in twisted graphene bilayers. *Physical Review B*. 92, 081406(R) (2015). doi:10.1103/PhysRevB.92.081406
- [4] L.-J. Yin; J.-B. Qiao; W.-X. Wang; W.-J. Zuo; W. Yan; R. Xu; R.-F. Dou; J.-C. Nie; L. He, Landau quantization and Fermi velocity renormalization in twisted graphene bilayers. *Physical Review B*. 92, 201408(R) (2015). doi:10.1103/PhysRevB.92.201408
- [5] L.-J. Yin; S.-Y. Li; J.-B. Qiao; J.-C. Nie; L. He, Landau quantization in graphene monolayer, Bernal bilayer, and Bernal trilayer on graphite surface. *Physical Review B*. 91, 115405 (2015). doi:10.1103/PhysRevB.91.115405
- [6] L.-J. Yin; W.-X. Wang; Y. Zhang; Y.-Y. Ou; H.-T. Zhang; C.-Y. Shen; L. He, Observation of chirality transition of quasiparticles at stacking solitons in trilayer graphene. *Physical Review B*. 95, 081402(R) (2017). doi:10.1103/PhysRevB.95.081402

**Session A2**

**14:30 - 15:00 PM Room A December 17**

**A04: Nuclear magnetic resonance in topological insulators:  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$**

A.O. Antonenko<sup>1,\*</sup>, E.V. Charnaya<sup>1</sup>, V.V. Marchenkov<sup>2,3</sup>, S.V. Naumov<sup>2</sup>

<sup>1</sup>*St. Petersburg State University, 1 Ulyanovskaya street, St. Petersburg, Russia*

<sup>2</sup>*M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, 18 S. Kovalevskaya street, Ekaterinburg, Russia*

<sup>3</sup>*Ural Federal University, 19 Mira street, Ekaterinburg, Russia*

\*Corresponding author. Email: nastya5555@mail.ru

**Abstract**

High quality single-crystalline topological insulators  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  were investigated by NMR in a large temperature range from 11 to 293 K. It was shown that NMR spectra for both compounds consisted of two lines which correlated to two nonequivalent positions of tellurium and selenium atoms in the crystallographic structures of  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$ , respectively. It was found for  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  single-crystalline plates that the less intensive line of the NMR spectra at room temperature began to dominate at low temperatures for the orientation when the crystallographic  $c$  axis was parallel to the external magnetic field  $\mathbf{B}_0$ . This behavior could not be explained with the angular dependence. The thermal-activation character of the temperature dependence of the Knight shift for the single-crystalline plate (when the  $c$  axis was perpendicular to  $\mathbf{B}_0$ ) and powder  $\text{Bi}_2\text{Te}_3$  was shown with activation energy 26 meV. The results provide information about electron-nuclear interactions in the materials studied. This could be useful for further theoretical and experimental studies of the electron properties in the three-dimensional topological insulators.

**Keywords**

Topological insulators (TIs); Nuclear magnetic resonance (NMR); Condensed matter physics; Low temperatures

**Session A2**

**15:00 - 15:30 PM Room A December 17**

**A05: Graphene Supported Graphone/Graphane Bilayer Nanostructure**

**Material for Spintronics**

Sekhar Chandra Ray\*

*Department of Physics, College of Science, Engineering and Technology, University of South Africa, Private Bag X6, Florida, 1710, Science Campus, Christiaan de Wet and Pioneer Avenue, Florida Park, Johannesburg, South Africa*

\*Corresponding author. Email: raysc@unisa.ac.za

**Abstract**

We have investigated the magnetic and electronic properties of partially hydrogenated vertically aligned few layers graphene (FLG) known as Graphone, synthesized by the microwave plasma enhanced chemical vapor deposition (PECVD). The FLGs are hydrogenated at different substrate temperatures to alter the degree of hydrogenation (Graphone/Graphane) and their depth profile. The unique morphology of the structure gives rise to a unique geometry in which Graphone/Graphane is supported by Graphene layers in the bulk, which is very different from other widely studied structures such as one-dimensional nanoribbons. Synchrotron based x-ray absorption fine structure spectroscopy measurements have been used to investigate the electronic structure and the underlying hydrogenation mechanism responsible for the magnetic properties. While ferromagnetic interactions seems to be predominant, the presence of antiferromagnetic interaction was also observed. Free spins available via the conversion of sp<sup>2</sup> to sp<sup>3</sup>-hybridized structures, and the possibility of unpaired electrons from defects induced upon hydrogenation are thought to be likely mechanisms for the observed ferromagnetic orders.

**References**

[1] Ray et al. 2014. Scientific Reports 4, 3862:1-7

**Session A3**

**16:00 - 16:30 PM Room A December 17**

**A06: Large positive magnetoresistance in twisted few layer graphene**

Oleg V. Kononenko<sup>1,2,\*</sup>, A.V. Zotov<sup>1</sup>, V.T. Volkov<sup>1</sup>, V.I. Levashov<sup>1</sup>, V.A. Tulin<sup>1</sup>, V.N. Matveev<sup>1</sup>

<sup>1</sup>*Affiliation Information Institute of Microelectronics Technology and High Purity Materials, Russian Academy of Sciences: 6, Academician Osipyan st., Chernogolovka, 142432, Moscow region, Russia*

<sup>2</sup>*National University of Science and Technology "MISIS": 4, Leninsky pr., Moscow, 119049, Russia*

\*Corresponding author. Email: oleg@iptm.ru

**Abstract**

Twisted or turbostratic bi- and multilayer graphene attracts much attention due to its unique properties [1-2]. Graphene films were grown on an iron film catalyst deposited on oxidized silicon substrate by the low-pressure chemical vapor deposition (LPCVD) method with a single injection of acetylene. Studies with the SENTERRA Bruker Raman microscope showed that the graphene films are a turbostratic few layer graphene. The electron transport and magnetotransport properties of the films were investigated. The temperature dependence of the graphene film resistance exhibits the thermally activated (TA) behavior at temperatures above 120° K. At lower temperature the dependence deviates from TA behavior and at temperatures below 40° K becomes close to the variable range hopping conduction. Unusually high positive magnetoresistance (MR) at a room temperature (100% in the magnetic field of 0.5 T) was found in the films. The MR was measured at different temperatures in the magnetic fields normal to the film plane. In low fields up to ~ 0.005 T at temperatures below ~ 40° K, negative MR was observed, caused by weak localization (WL). In magnetic fields above ~ 0.005 T, the MR increases with increasing magnetic field and becomes positive with quadratic magnetic-field dependence in the fields up to ~ 0.03 T and quasi linear dependence in the fields higher than ~ 0.03 T.

**Keywords**

Twisted few layer graphene; CVD; electrical transport; magnetoresistance

**Acknowledgements**

O.V.K. gratefully acknowledge the financial support of the Ministry of Education and Science of the Russian Federation in the frame-work of Increase Competitiveness Program of NUST «MISIS» (grant K2-2017-009).

**References**

- [1] T.-F. Chung, Y. Xu, Y. P. Chen, Transport measurements in twisted bilayer graphene: Electron-phonon coupling and Landau level crossing. *Phys. Rev. B* 98, 035425 (2018). doi:10.1103/PhysRevB.98.035425
- [2] U. Mogera, S. Walia, B. Bannur, M. Gedda, G. U. Kulkarni, Intrinsic Nature of Graphene Revealed in Temperature Dependent Transport of Twisted Multilayer Graphene. *J. Phys. Chem. C*, 121, 13938 (2017). doi: 10.1021/acs.jpcc.7b04068

**Session A3**

**16:30 - 17:00 PM Room A December 17**

**A07: Graphene nanotubes reinforced aluminum based superprofile**

Hansang Kwon<sup>1,2,\*</sup>, Kyungju Kim<sup>1,2</sup>

<sup>1</sup>*Pukyong national University:45Yongso-ro, Nam-Gu, Busan, 48513, Republic of Korea*

<sup>2</sup>*Next Generation Materials Co., Ltd.: 365Sinseon-ro, Namgu, Busan, 48547, Republic of Korea*

\*Corresponding author. Email: kwon13@pknu.ac.kr

**Abstract**

Single walled carbon nanotubes (SWCNT) or graphene nanotubes was mixed with aluminum powders by mechanical ball milling and the composite powders was directly extruded after special billet preparation [1]. The superprofile was successfully fabricated the combination of the Al and graphene nanotubes by a hot extrusion [2] process as a world first. It specially the superprofiles could be used for composed of various frame elements and brackets needed for assembling with T-slot structure which has advantage of no welding, simple designed, short manufacturing time and easy to recycling and so on. The superprofile was combined with nano and micro sized powder and microstructure [3]. The mechanical properties were increased than that of general Al profile, especially young's modulus was 3times higher than that of Al. It is possible to use for many automation system frame, electric vehicle parts and customized solar battery frame and so on.

**Keywords**

Single walled carbon nanotubes (SWCNT); Graphene nanotubes; Aluminum; Profile; Extrusion

**References**

- [1] H. Kwon; M. Estili; K. Takagi; T. Miyazaki; A. Kawasaki, Combination of hot extrusion and spark plasma sintering for producing carbon nanotube reinforced aluminium matrix composites. *Carbon*. 47, 570 (2009). doi.org/10.1016/j.carbon.2008.10.041
- [2] H. Kwon; M. Laparoux. Hot extruded carbon nanotube reinforced aluminium matrix composite materials. *Nanotechnology*. 23, 415701 (2016). doi:10.1088/0957-4484/23/41/415701
- [3] H. Kurita; H. Kwon; M. Estili; A. Kawasaki. Multi-walled carbon nanotube-aluminum matrix composites prepared by combination of hetero-agglomeration method, spark plasma sintering and hot extrusion. *Materials Transactions*. 52, 1960 (2011). doi:10.2320/matertrans.M2011146



**Session A3**

**17:00 - 17:30 PM Room A December 17**

**A08: Electron emission theories for 2D-materials and applications**

L. K. Ang\*, Y. S. Ang

*Science and Mathematics, Singapore University of Technology and Design, Singapore*

\*Corresponding author. Email: ricky\_ang@sutd.edu.sg

**Abstract**

Electron emission from a material through an interface such as vacuum or another material is a fundamental process in cathode, diode, ionization, electric contact and many other areas. Depending on the energy used for electron emission, it can be broadly characterized into 3 different processes known as thermionic emission TE (by thermal energy), field emission FE (by quantum tunneling) and photoemission PE (by absorption of photons or optical tunneling). The basic models for these processes (TE, FE, PE) have been formulated many decades ago, respectively, known as the Richardson law, Fowler-Nordheim (FN) law, and photo-electric effect or Keldysh model. At high current regime, the emission laws will become space charge limited, which is known as Child-Langmuir (CL) law and Mott-Gurney (MG) law for vacuum gap and solid-diode respectively. With the development of two-dimensional (2D) atomic scale materials in the 2000's, the above-mentioned classical laws may require revisions to account for new material properties, as well as novel operating regimes in nanometer dimensions and in ultrashort time scales. In this presentation, we will present some recent and self-consistent emission models [1-6] to illustrate that the classical laws are no longer valid for 2D materials such as graphene. These new models exhibit smooth transition to the classical models and provides new scaling laws due to the unique properties of 2D materials. Comparison with some experimental results will be discussed. Some selected applications of these models on areas such as energy harvesting, electronics and material characterization.

**Keywords**

2D materials; interface physics; emission models; nano-electronics; modeling

**References**

- [1] Y. S. Ang, H. Y. Yang, and L. K. Ang, "Universal scaling in nanoscale lateral Schottky heterostructures", *Phys. Rev. Lett.* 121, 056802 (2018). doi: 10.1103/PhysRevLett.121.056802
- [2] Y. S. Ang, S. J. Liang, and L. K. Ang, "Theoretical Modelling of Electron Emission from Graphene", *MRS Bulletin* 42, 505 (2017). doi: 10.1557/mrs.2017.141
- [3] Y. S. Ang, M. Zubair, and L. K. Ang, "Relativistic space charge limited current for massive Dirac fermions", *Phys. Rev. B* 95, 165409 (2017). doi: 10.1103/PhysRevB.95.165409
- [4] Shijun Liang, Bo Liu, Wei Hu, Kun Zhou and L. K. Ang, "Thermionic Energy Conversion Based on Graphene van der Waals Heterostructures", *Scientific Report* 7:46211 (2017). doi: 10.1038/srep46211
- [5] Y. S. Ang, and L. K. Ang, "Current-temperature scaling for a Schottky interface with non-parabolic energy Dispersion", *Phys. Rev. Applied* 6, 034013 (2016). doi: 10.1103/PhysRevApplied.6.034013
- [6] Shijun Liang, and L. K. Ang, "Electron Thermionic Emission from Graphene and thermionic energy convertor", *Phys. Rev. Applied* 3, 014002 (2015). doi: 10.1103/PhysRevApplied.3.014002

**Session A3**

**17:30 - 18:30 PM Room A December 17**

## A09: Graphene nanoribbons formed by a sonochemical graphene unzipping using supramolecular template

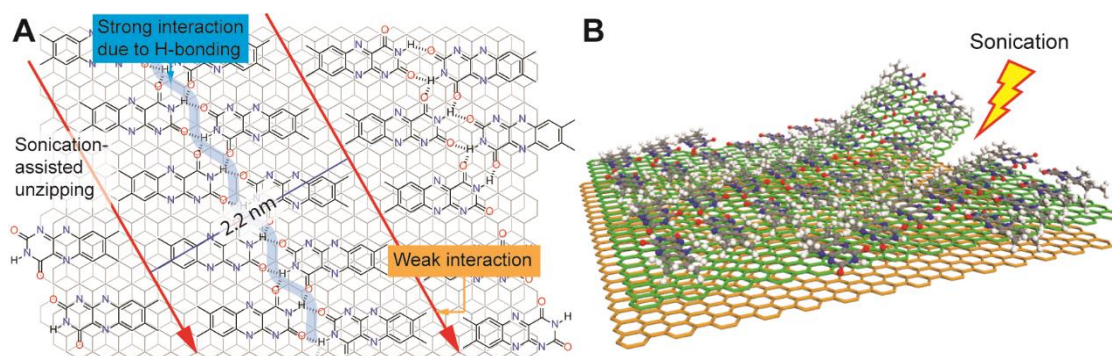
Sang-Yong Ju\*

*Department of Chemistry, Yonsei University, Republic of Korea*

\*Corresponding author. Email: syju@yonsei.ac.kr

### Abstract

When the width of a graphene nanoribbon (GNR) is below 10 nm, it possesses semiconducting properties that enable various high-end electronic applications. Here, we report that the dense and stable dispersion of a natural graphite flake by using flavin mononucleotide (FMN) as a surfactant produces GNRs as small as 10 nm in width. High-resolution transmission electron microscopy reveals GNRs with various widths, along with a graphene flake containing straight-edged GNRs and cuts. GNR formation originates from sonochemical graphene unzipping along a one-dimensional FMN supramolecular template. Various Raman methods demonstrate the universal intensity ratio of D over D' bands near 4, supporting formation of continuous edge defect. Thermal annealing enhances the optical contrast and van der Waals interactions of the graphene film, resulting in increased conductivity compared to the as-prepared graphene film, which is also better than that of reduced graphene oxide.



**Keynote Talk**

**9:00 - 9:45 AM Room B December 17**

## **K03: Synthesis of Two Different Types of Phase-selectively Disordered Blue TiO<sub>2</sub> Nanomaterials and their Applications**

Hyoyoung Lee<sup>1,2,3,4,\*</sup>

<sup>1</sup>Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Sungkyunkwan University, Suwon, 16419, Republic of Korea

<sup>2</sup>Department of Chemistry, <sup>3</sup>Department of Energy Science and <sup>4</sup>Department of SAINT, Sungkyunkwan University (SKKU), Suwon, 16419, Republic of Korea

\*Corresponding author. Email: hyoyoung@skku.edu

### **Abstract**

A low energy absorbed semiconducting materials has been sought for a long time for the visible light-driven photocatalytic reactions. To prepare the low energy absorbed semiconducting materials such as TiO<sub>2</sub>, various types of low energy band gap TiO<sub>2</sub> materials have been introduced. Most low energy band gap TiO<sub>2</sub> materials such as black TiO<sub>2</sub> has a large amount of phase-disordered defect sites. The phase-disordered defects can efficiently absorb the visible light but also are served as charge recombination sites of the electrons and holes produced under light irradiation. This charge recombination decreases an efficiency for any kinds of devices and systems. Therefore, it is quite necessary to find new semiconducting nanomaterials that have a disordered TiO<sub>2</sub> phase for the light absorption as well as a crystalline phase for the fast charge separation within a nanometer scale. Here, we report novel synthesis method for the phase-selectively disordered, rutile-only phase in a phase-mixed P25 TiO<sub>2</sub> (ordered anatase and disordered rutile, OA/DR) and anatase-only phase in a phase-mixed P25 TiO<sub>2</sub> (disordered anatase and ordered rutile, DA/OR), which are produced via alkali metal-liquid ammonia treatments under room temperature and ambient atmosphere in solution. The strong advantage of phase selective reduction method can allow to control an active site where Ti<sup>3+</sup> is generated while keeping the other crystalline phase. Both resulting blue colored TiO<sub>2</sub> (HYL' s blue TiO<sub>2</sub>) nanomaterials shows a high light absorption including visible light and simultaneously high charge transport ability that is confirmed by photoluminescence light measurement. For a possible application, we like to introduce new findings about hydrogen evolving reaction (HER) [1], removal of algae from water [2], visible light-driven CO<sub>2</sub> reduction, decomposition of organic compounds and particle matters, and etc.

### **Keywords**

Phase-selective reduction; Blue TiO<sub>2</sub>; Hydrogen evolution reaction (HER); Organic compound and particle matter's decomposition; CO<sub>2</sub> reduction

### **References**

- [1] Kan Zhang et al. An order/disorder/water junction system for highly efficient co-catalyst-free photocatalytic hydrogen generation, *Energy & Environmental Science* 2016, 9, 499-503
- [2] Youngmin Kim et al. Solar-light photocatalytic disinfection using crystalline/amorphous low energy bandgap reduced TiO<sub>2</sub>, *Scientific Reports*, 2016, 6, 25212; doi: 10.1038/srep25212

**Keynote Talk**

**9:45 - 10:30 AM Room B December 17**

## **K04: Highly Efficient Photoconversion of CO<sub>2</sub>: Controllable Transition from C1 to C2 Products**

Su-il In\*

*Department of Energy Science and Engineering, DGIST, Republic of Korea*

\*Corresponding author. Email: insuil@dgist.ac.kr

### **Abstract**

Photocatalytic reduction of CO<sub>2</sub> to fuel offers an exciting opportunity for helping to solve current energy and global warming problems. Although a number of solar active catalysts have been reported, most of them suffer from low product yield, instability, and low quantum efficiency. Therefore, the design and fabrication of highly active photocatalysts remains an unmet challenge. We seek CO<sub>2</sub> photoconversion efficiencies large enough for translation of the technology from laboratory to industry, a key step of which is achieving higher-order hydrocarbon products. Ethane, C<sub>2</sub>H<sub>6</sub>, for example, can be relatively easily converted into ethanol, a liquid fuel. In the current work, under AM1.5G illumination, utilizing a photocatalyst of reduced titania, graphene, and Pt nanoparticles, we demonstrate stable operation, significant rates of product formation, as well as a controllable product transformation from CH<sub>4</sub> to C<sub>2</sub>H<sub>6</sub>. We find the switch from C1 to C2 products is dependent upon upward band bending at the reduced blue-titania/graphene interface.

### **References**

- [1] Saurav Sorcar, Jamie Thompson, Yunju Hwang, Young Ho Park, Tetsuro Majima, Craig A. Grimes, James R. Durrant\* and Su-il In\*, "High-Rate Solar-spectrum Photoconversion of CO<sub>2</sub>: Controllable Transition from C1 to C2 Products", *Energy & Environmental Science* 11 (2018) 3183-3193
- [2] Muhammad Zubair, Hye Rim Kim, Abdul Razzaq, Craig A. Grimes, and Su-il In\*, "Solar spectrum photocatalytic conversion of CO<sub>2</sub> to CH<sub>4</sub> utilizing TiO<sub>2</sub> nanotube arrays embedded with graphene quantum dots", *Journal of CO<sub>2</sub> Utilization* 26 (2018) 70-79
- [3] Abdul Razzaq, Apurba Sinhamahapatra, Tong-Hyung Kang, Craig A. Grimes, Jong-Sung Yu\* and Su-il In\*, "Efficient Solar Light Photoreduction of CO<sub>2</sub> to Hydrocarbon Fuels via Magnesiumthermally Reduced TiO<sub>2</sub> Photocatalyst", *Applied Catalysis B* 215 (2017) 28-35
- [4] Hye Rim Kim, Abdul Razzaq, Craig A. Grimes, and Su-II In\*, "Synthesis of Heterojunction p-n-p Cu<sub>2</sub>O/S-TiO<sub>2</sub>/CuO, and Application to the Photocatalytic Conversion of CO<sub>2</sub> and Water Vapor to Methane", *Journal of CO<sub>2</sub> Utilization* 20 (2017) 91-96
- [5] Saurav Sorcar, Yunju Hwang, Craig A. Grimes, and Su-il In\*, "Highly Enhanced and Stable Activity of Defect Induced Titania Nanoparticles for Solar Light Driven CO<sub>2</sub> Reduction into CH<sub>4</sub>", *Materials Today* Volume 20, Issue 9 (Nov. 2017) 507-51

**Session B1**

**11:00 - 11:30 AM Room B December 17**

**B01: Effective solar energy conversion based on spectral control of thermal radiation via monolithic absorber/emitter**

Makoto Shimizu\*, Asaka Kohiyama, Kana Konno, Hiroo Yugami

*Tohoku University, Japan*

\*Corresponding author. Email: m\_shimizu@energy.mech.tohoku.ac.jp

**Abstract**

In this presentation, we will introduce the effective solar energy conversion technology using thermophotovoltaic (TPV) systems. In TPV systems, thermal radiation from the heated material is converted into electricity by photovoltaic (PV) cells. The systems that use concentrated solar energy as a heat source is especially called as solar-TPV systems which is recently attract much attention [1-3]. In this system, solar energy can be converted into useful thermal radiation by a monolithic absorber/emitter. Most of photon energy of sunlight can be turned into heat at the absorber and then the monolithic emitter emits the useful photon of which energy is above the bandgap of the PV cells. Efficiency of a solar-TPV system, therefore, can be expected to reach close to 45% [4] even with single-junction cells.

At first, we will explain a result of a solar-TPV system's design. Total efficiency of solar-TPV systems can be described with two types of efficiencies such as the extraction efficiency  $\eta_{\text{extract}}$  and the PV cell conversion efficiency  $\eta_{\text{PV}}$  [5]. The  $\eta_{\text{extract}}$  expresses how effectively solar energy is converted into thermal radiation power from the emitter. The  $\eta_{\text{PV}}$  shows how effectively the thermal radiation power is converted into electric energy. To achieve high efficiency, spectral shaping of thermal radiation from absorber and emitter is essential. Geometric design such as the absorber/emitter shape and configuration of each component is also important.

We will also show experimental results of the spectral shaping of thermal radiation using metal-dielectric layered structure. A solar-TPV system is usually working at very high-temperature (>1000 °C) to have high  $\eta_{\text{PV}}$ . Therefore, both high spectral selectivity and high thermal stability are required for the structure. It is revealed that the layered structure composed of molybdenum nanometric film sandwiched by hafnium oxide layer shows high spectral selectivity and is thermally stable up to 1150 °C [6].

Finally, we will represent results of power generation tests using high power density solar simulator. Gallium antimonide cell which have a band gap of 0.67 eV is used as a PV cell. Two shapes of the monolithic absorber/emitter such as planar type and cube type system are demonstrated in the tests. In both test, total efficiency reach to more than 5%.

**Keywords**

Thermophotovoltaics; Solar; Thermal radiation; Spectral shaping; Gallimu antimonide cells

**References**

- [1] A. Datas; C. Algora, Development and experimental evaluation of a complete solar thermophotovoltaic system. *Progress in Photovoltaics*. 21(5), 1025-1039 (2013). doi: 10.1002/pip.2201
- [2] M. Shimizu; A. Kohiyama; H. Yugami, High-efficiency solar-thermophotovoltaic system equipped with a monolithic planar selective absorber/emitter. *Journal of Photonics for Energy*. 5(1), 053099 (2015). doi: 10.1117/1.JPE.5.053099

- [3] D. M. Bierman; A. Lenert; W. R. Chan; B. Bhatia; I. Celanović; M. Soljačić; E. N. Wang, Enhanced photovoltaic energy conversion using thermally based spectral shaping. *Nature Energy*. 1, 16068 (2016). doi: 10.1038/nenergy.2016.68
- [4] A. Datas; C. Algora, Detailed balance analysis of solar thermophotovoltaic systems made up of single junction photovoltaic cells and broadband thermal emitters. *Solar Energy Materials and Solar Cells*. 94(12), 2137-2147 (2010). doi: 10.1016/j.solmat.2010.06.042
- [5] A. Kohiyama; M. Shimizu; H. Yugami, Unidirectional radiative heat transfer with a spectrally selective planar absorber/emitter for high-efficiency solar thermophotovoltaic systems. *Applied Physics Express*. 9(11), 112302 (2016). doi: 10.7567/APEX.9.112302
- [6] M. Shimizu; A. Kohiyama; H. Yugami, Evaluation of thermal stability in spectrally selective few-layer metallo-dielectric structures for solar thermophotovoltaics. *Journal of Quantitative Spectroscopy and Radiative Transfer*. 212, 45-49 (2018). doi: 10.1016/j.jqsrt.2018.02.037

**Session B1**

**11:30 - 12:00 PM Room B December 17**

**B02: MoS<sub>2</sub>-based electrocatalysts for hydrogen evolution catalysis: a comparative study on synthesis methods**

Seokhee Shin, Zhenyu Jin, So-Yeon Ham, Suhyun Lee, Dasom Shin, Yo-Sep Min\*

*Department of Chemical Engineering, Konkuk University, 120 Neungdong-Ro, Gwangjin-Gu, Seoul 05029, Republic of Korea*

\*Corresponding author. Email: ysmin@konkuk.ac.kr

**Abstract**

Molybdenum disulfide (MoS<sub>2</sub>) is one of promising catalysts for hydrogen evolution reaction. In the 2H structure of MoS<sub>2</sub>, which is one of layered transition metal chalcogenides, basal planes are electrochemically inactive but its edge sites are active for the HER catalysis. Various strategies such as doping, vacancy engineering, and structural engineering have been extensively investigated to activate the basal planes and/or to improve the HER activity. Recently, it is reported that amorphous molybdenum sulfide (a-MoS<sub>x</sub>) has a high active site density due to the presence of disorderly-arranged atoms unlike crystalline MoS<sub>2</sub>. Furthermore, isotropic electrical conductivity of the a-MoS<sub>x</sub> is much more advantageous to the electron transfer for the HER, comparing to the anisotropic conductivity of the crystalline MoS<sub>2</sub>. [1] Here, we report an amorphous catalyst of oxygen-incorporated molybdenum sulfide (a-MoO<sub>x</sub>S<sub>y</sub>) synthesized at 90 °C on carbon fiber paper (CFP) by chemical bath deposition (CBD) method. Ammonium heptamolybdate and thioacetamide were used as molybdenum and sulfur precursors, respectively. Sodium dithionite was added to the precursor solution as a reducing agent to adjust the oxygen content and oxidation states of molybdenum and sulfur ions. The HER performance of a-MoO<sub>x</sub>S<sub>y</sub> is much more excellent than that of a-MoS<sub>x</sub> without any incorporated oxygen. The high activity of a-MoO<sub>x</sub>S<sub>y</sub> is strongly related to the oxidation states of molybdenum and sulfur ions. [2] The importance of the oxidation state will be discussed by comparing activities of various amorphous catalysts previously reported by using atomic layer deposition [1, 3] and hydrothermal method [4, 5].

**Keywords**

Molybdenum sulfide; oxygen incorporation; oxidation state; hydrogen evolution reaction

**References**

[1] S. Shin; Z. Jin; D. H. Kwon; R. Bose; Y. Min, *Langmuir*. 31, 1196-1202 (2015).

Doi:10.1021/la504162u

[2] P. D. Tran; T. V. Tran; M. Orio; S. Torelli; Q. D. Truong; K. Nayuki; Y. Sasaki; S. Y. Chiam; R. Yi, I. Honma; J. Barber; V. Artero, *Nature materials*, 15, 640-646 (2016). Doi:10.1038/NMAT4588

[3] D.H. Kwon; Z. Jin; S. Shin; W. Lee; Y. Min, *Nanoscale*. 8, 7180-7188 (2016).

Doi:10.1039/c5nr09065b

[4] R. Bose; S. K. Balasingam; S. Shin; Z. Jin; D. H. Kwon; Y. Jun; Y Min, *Langmuir*. 31, 5220-5227 (2015).

Doi:10.1021/acs.langmuir.5b00205

[5] R. Bose; Z. Jin; S. Shin; S. Kim; S. Lee; Y. Min; *Langmuir*. 33, 5628-5635 (2017).

Doi:10.1021/acs.langmuir.7b00580

**Session B1**

**12:00 - 12:30 PM Room B December 17**

**B03: Novel concept of intermediate band for III-V Nitride solar cells**

Liwen Sang\*, Meiyong Liao, Masatomo Sumiya

*International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Ibaraki, Japan*

\*Corresponding author. Email: SANG.Liwen@nims.go.jp

**Abstract**

III-Nitride semiconductor  $\text{In}_x\text{Ga}_{1-x}\text{N}$  has the unique advantage of the widest adjustment of direct bandgaps from infrared (InN at 0.65 eV) to ultraviolet (UV) (GaN at 3.42 eV) region. Compared with Si, GaAs, CuInGaSe or Ge systems, it is the only semiconductor system that can provide the perfect match to the solar spectrum. On the other hand, InGaN-based alloys also have the favorable physical properties of high absorption coefficient ( $\sim 10^5\text{cm}^{-1}$ ), high radiation resistance, high drift velocity, and high carrier mobility. The theoretical power conversion efficiency of a four-junction solar cell based on InGaN is expected to be more than 50% according to the balance modeling estimation. However, creating high-quality InGaN alloys with this wide range of energy bandgap for photovoltaic application remains a challenge.

In this paper, we propose a novel concept of intermediate-band (IB) transition to the InGaN-based p-n junctions, and demonstrated the first IB solar cells from deep UV to near infrared region by InGaN/GaN multi-level quantum dots (QDs). The multiple IB by embedding a high-quality multi-stacked InGaN/GaN QDs into on p-n junction was demonstrated on AlN/sapphire template. The quantum confinement in the QDs leads to the splitting of the energy levels and the coupling among the QDs forms the three-dimensional minibands. The short-circuit current density of the solar cell is greatly improved. The intermediate band transitions are confirmed and further discussed with regard to the device physics.

**Keywords**

Intermediate band; solar cells; III-V nitrides; InGaN; quantum dots

**References**

[1] L. Sang, M. Liao, Q. Liang, M. Takeguchi, B. Dierre, B. Shen, T. Sekiguchi, Y. Koide, and M. Sumiya, *Adv. Mater.*, 26, 1414-1420(2014)



**Session B2**

**14:00 - 14:30 PM Room B December 17**

**B04: A high throughput synthesis of semiconductor nanocrystals and preparation of highly luminescent composite beads for LEDs**

Young-Kuk Kim\*

*Dept. of functional powders, Korea Institute of Materials Science (KIMS): #797 Changwondaero, Changwon, Kyungnam, Republic of Korea*

\*Corresponding author. Email: voice21@kims.re.kr

**Abstract**

Highly luminescent quantum dots (QDs) with narrow emission spectra were continuously synthesized with a fluid dynamically controlled reactor. Here, we developed a continuous synthesis method for QDs based on Taylor-Couette reactor (TCR). Stable continuous synthesis process was achieved after 20 minutes from the start of continuous injection of precursors and the measured standard deviation of wavelength and width of emission spectra was less than 1nm. As a result, high space-time yield of 1kg/hour-liter was achieved for synthesis of highly quality QDs. Near unity quantum yield (~ 0.9) was demonstrated after surface capping of TCR-processed cores with CdS. The prepared CdSe/CdS QDs showed intense photoluminescence at 645nm with a spectral linewidth of 35nm, which is much narrower than PL spectra of QDs synthesized from conventional batch-type synthesis route using reaction vessel with large volume capacity. Polymer beads containing highly luminescent QDs were prepared by “bead in bead” configuration via swelling of polymer beads and subsequent adsorption of QDs. After in-situ surface coating with aluminosilicates exceptional stability was attained even under irradiation of ultraviolet light and presence of ozone.

**Keywords**

Quantum dots; Core-shell structure; polymer beads; Quantum yield; Continuous synthesis

**References**

- [1] Y. K. Kim, S. H. Ahn, K. Chung, Y. S. Cho, C. J. Choi, The photoluminescence of CuInS<sub>2</sub> nanocrystals: effect of non-stoichiometry and surface modification, *J. Mater. Chem.*, 2012,22, 1516-1520, DOI: 10.1039/C1JM13170B
- [2] W. K. Bae, K. Char, H. Hur, S. Lee, Single-step synthesis of quantum dots with chemical composition gradients, *Chem. Mater.* 2008, 20, 2, 531-539, DOI: 10.1021/cm070754d

**Session B2**

**14:30 - 15:00 PM Room B December 17**

**B05: Two-dimensional semiconductor based transparent solar cell and its performance enhancement**

Ah-Jin Cho<sup>1,2</sup>, Min-Kyu Song<sup>1,2</sup>, Dong-Won Kang<sup>3</sup>, Jang-Yeon Kwon<sup>1,2,\*</sup>

<sup>1</sup>*School of Integrated Technology, Yonsei University, Songdogwahak-ro 85, Incheon, 21983, Republic of Korea*

<sup>2</sup>*Yonsei Institute of Convergence Technology, Songdogwahak-ro 85, Incheon, 21983, Republic of Korea*

<sup>3</sup>*School of Energy Systems Engineering, Chung-Ang University, Heukseok-ro 84, Seoul, 06974, Republic of Korea*

Email: ahjincho@yonsei.ac.kr (Ah-Jin Cho)

**Abstract**

As a means to overcome the limitation of installation space and to promote the utilization of the solar cell in various applications, a transparent thin-film solar cell has been studied by many researchers [1-2]. To achieve a transparent solar cell, the choice of materials which are transparent enough and showing the photovoltaic property at the same time is the key. Here, we suggest a two-dimensional (2D) p-n heterojunction of WSe<sub>2</sub>/MoS<sub>2</sub> and an Indium tin oxide (ITO) electrode to fabricate a transparent thin-film photovoltaic cell. Due to advantages that 2D materials possess [3-4], a highly transparent (~80 %) solar cell with considerable efficiency was achieved. Furthermore, by introducing a transparent passivation layer composed of a fluoropolymer, the photovoltaic performance was much improved. With the passivation layer, our WSe<sub>2</sub>/MoS<sub>2</sub> transparent photovoltaic cell reached an efficiency of ~10 %. Comparison of photovoltaic parameters before and after applying passivation and analysis on the origin of such differences will be also presented. To the best of our knowledge, we are the first group to fabricate a 2D material-based fully transparent photovoltaic device. Our result exhibits a great potential of the van der Waals (vdW) p-n heterojunction of 2D semiconductors to be utilized for an active layer of a highly transparent and light-weighted thin-film solar cell.

**Keywords**

Transparent solar cell; 2D semiconductor; van der Waals heterostructure; fluoropolymer; p-n junction

**Session B2**

**15:00 - 15:30 PM Room B December 17**

**B06: Modulation by modelling of the morphology of (nano) micromaterials**

Amanda F. Gouveia<sup>1,\*</sup>, Elson Longo<sup>1</sup>, Juan Andrés<sup>2</sup>

<sup>1</sup>Federal University of São Carlos: P.O. Box 676, São Carlos, Brazil

<sup>2</sup>University Jaume I: Street de Vicent Sos Baynat, Castelló, Spain

\*Corresponding author. Email: amanda@liec.ufscar.br

**Abstract**

Experiment and theoretical researchers often asked themselves if ‘Can they believe modelling?’. Answering it requires informed understanding of the strengths and limitations of both current computational modelling and simulation methods as well as experimental techniques and their ranges of application. It is mandatory to enter a self-critical dialogue between theory and experiment rather than to do either theory or experimental in isolation and put unconditional trust in the results of such studies. This is a fertile and growing area, with exciting opportunities and an enormous range of potential applications. It is crucial for the modeler in nanotechnology and materials science to understand the issues of interest to experimentalists, the complexity of chemical systems and how to tackle them effectively by modelling.

In our case, the modulation of the morphologies of (nano) micromaterials imply the joint the use of the first principles to calculate the most stable surfaces and the Wulff construction and the screening of the relative values of surface energies of exposed facets. Analyzing this procedure, we can propose how reach a desired morphology and the pathway linking the ideal (more stable) to the experimental observed morphology. Then, it is possible to understand and rationalize the morphology evolution process, i.e. the modulation process.

In this study, it was investigated the influence of a surfactant anionic and the temperature during the synthesis process of  $\alpha$ -Ag<sub>2</sub>WO<sub>4</sub> and ZnWO<sub>4</sub>, respectively, and their facet-dependent photocatalytic activities are unraveled.

**Keywords**

1. To provide scientific guidance for morphological control of (nano)micromaterial synthesis
2. An analysis of how the idealized in vacuo surface results can be related to the in situ behavior
3. This study provides new insights into the crystal growth habit and morphology transformation
4. To develop a programmable 3D chemical shaping strategy for morphology modulation based on the Wulff construction
5. This new strategy not only decouples the degree of shape complexity from the production costs and time, but also enables a versatile, low-cost, scalable process for 3D shaping of diverse materials, which could lead to new material functions and applications

**Session B3**

**16:00 - 16:30 PM Room B December 17**

**B07: Black liquor-derived porous carbons from rice straw for high-performance supercapacitors**

Xinhua Qi\*, Linfeng Zhu, Feng Shen

*Agro-Environmental Protection Institute, Chinese Academy of Agricultural Sciences, No. 31, Fukang Road, Nankai District, Tianjin 300191, China*

\*Corresponding author. Email: qixinhua@nankai.edu.cn

**Abstract**

Supercapacitors are energy storage devices that retain electrical charge by an electrostatic double-layer or through electrochemical pseudocapacitance and have high power density and charge-discharge rates and their longer lifetime compared with traditional energy storage devices [1-3]. Activated carbons are widely used to prepare electrode materials due to their large surface area and relatively low cost [4]. In this work, rice straw was pretreated with KOH aqueous solution and the resulting liquid was used to synthesize a black liquor-derived porous carbon (BLPC) in which KOH acts as both lignin extraction solvent and chemical activation agent. The addition of melamine into the black liquor led to an increase in the surface area ( $2646 \text{ m}^2 \cdot \text{g}^{-1}$ ), pore volume ( $1.285 \text{ cm}^3 \cdot \text{g}^{-1}$ ) and promoted the formation of nitrogen covalent bonds in the carbon materials (N-BLPC). Melamine used as additive has dual roles as nitrogen source and pore modifier of the carbon material. The as-prepared materials had specific capacitances of  $242 \text{ F} \cdot \text{g}^{-1}$  (BLPC) and  $337 \text{ F} \cdot \text{g}^{-1}$  (N-BLPC) when used as electrodes in 6 M KOH electrolyte at a current density of  $0.5 \text{ A} \cdot \text{g}^{-1}$ . The assembled N-BLPC-based symmetric supercapacitor showed stable cycling ( $>98 \%$  retention after 3000 cycles at  $10 \text{ A} \cdot \text{g}^{-1}$ ). The proposed strategy offers a facile method to produce porous carbons from waste black liquor in biorefinery or pulp and paper processes, which has potential applications for adsorption, catalysis and energy storage.

**Keywords**

Supercapacitor; biomass; lignin; black liquor; carbon

**References**

- [1] J.R. Miller; P. Simon, Electrochemical capacitors for energy management, *Science* 321, 651 (2008). Doi:10.1126/science.1158736
- [2] T. Lin; I.W. Chen; F. Liu; C. Yang; H. Bi; F. Xu; F. Huang, Nitrogen-doped mesoporous carbon of extraordinary capacitance for electrochemical energy storage, *Science* 350, 1508 (2015). doi: 10.1126/science.aab3798
- [3] H.S. Huang; K.H. Chang; N. Suzuki; Y. Yamauchi; C.C. Hu; K.C. Wu, Evaporation-induced coating of hydrous ruthenium oxide on mesoporous silica nanoparticles to develop high-performance supercapacitors, *Small* 9, 2520 (2013). doi: 10.1002/sml.201202786
- [4] M. Sevilla; R. Mokaya, Energy storage applications of activated carbons: supercapacitors and hydrogen storage, *Energy & Environmental Science* 7, 1250 (2014). doi: 10.1039/c3ee43525c

**Session B3**

**16:30 - 17:00 PM Room B December 17**

**B08: Making structured metals transparent for broadband electromagnetic waves**

Lu Gan\*

*National Laboratory of Solid State Microstructures, School of Physics, and Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China*

\*Corresponding author. Email: ganlu@njfu.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.

**References**

- [1] X. R. Huang, R. W. Peng, and R. H. Fan, "Making metals transparent for white light by spoof surface plasmons", *Phys. Rev. Lett.* 105, 243901 (2010)
- [2] R. H. Fan, R. W. Peng, X. R. Huang, J. Li, Y. Liu, Q. Hu, Mu Wang, and X. Zhang, "Transparent metals for ultrabroadband electromagnetic waves", *Adv. Mater.* 24, 1980 (2012)
- [3] R. H. Fan, J. Li, R. W. Peng, X. R. Huang, D. X. Qi, D. H. Xu, X. P. Ren, and Mu Wang, "Oblique metal gratings transparent for broadband terahertz waves", *Appl. Phys. Lett.* 102, 171904 (2013)
- [4] R. H. Fan, L. H. Zhu, R. W. Peng, X. R. Huang, D. X. Qi, X. P. Ren, Q. Hu, and Mu Wang, "Broadband antireflection and light-trapping enhancement of plasmonic solar cells", *Phys. Rev. B* 87, 195444 (2013)
- [5] X. P. Ren, R. H. Fan, R. W. Peng, X. R. Huang, D. H. Xu, Y. Zhou, and Mu wang, "Nonperiodic metallic gratings transparent for broadband terahertz waves", *Phys. Rev. B* 91, 045111 (2015)

**Session B3**

**17:00 - 17:30 PM Room B December 17**

**B09: Electron transport characteristics of films comprised of transparent conducting nanocrystals synthesized by plasma**

Elijah Thimsen\*

*Institute for Material Science and Engineering, Department of Energy, Environmental and Chemical Engineering, Washington University in Saint Louis, USA*

\*Corresponding author. Email: elijah.thimsen@wustl.edu

**Abstract**

Transparent conducting oxide (TCO) thin films comprised of heavily doped wide-gap semiconductors are a ubiquitous feature of modern optoelectronics such as flat panel displays and touch screens. TCO materials also find application in thin film photovoltaic devices wherein charge carriers must be collected in the direction of the substrate surface normal. For the solar energy harvesting application, which is high volume and low margin, production cost is a key technology driver. Thus thin films comprised of TCO nanocrystals have attracted attention because they can be deposited at very high rates and relatively low cost by aerosol or solution phase processing. Among the two material properties that determine the figure of merit for a TCO, namely the light transmission and electrical conductivity, achieving facile charge carrier transport has proved to be much more difficult. In this talk, I will discuss the chemical and structural characteristics that are required for achieving high electrical conductivity in thin films comprised of TCO nanocrystals synthesized by plasma. The talk will focus primarily on results related to our work on ZnO. More recently, we have begun to focus on SnO<sub>2</sub>. SnO<sub>2</sub> is much more chemically robust compared to ZnO and therefore finds a broader class of applications (e.g. electrochemical). A quantitative framework for describing the relationship of structure to electrical conductivity for thin films comprised of nanocrystals will be presented that is based on classical percolation theory and also incorporates aspects of state-of-the-art electron transport theory.

**Session B3**

**17:30 - 18:00 PM Room B December 17**

## **B10: Noble photocatalytic systems for degradation and detection of pollutants towards wastewater treatment applications**

Narendra Singh<sup>1</sup>, Pratyush Jain<sup>1</sup>, Ankit Tyagi<sup>1</sup>, Prasenjit Kar<sup>1</sup>, Jai Prakash<sup>1</sup>, Raju Kumar Gupta<sup>1,2,\*</sup>

<sup>1</sup>Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India

<sup>2</sup>Center for Nanosciences and Center for Environmental Science and Engineering, Indian Institute of Technology Kanpur, Kanpur, India

\*Corresponding author. Email: guptark@iitk.ac.in

### **Abstract**

Water pollution is an emerging problem across the world due to rapid population growth and modern industrialization. Waste water contains organic (such as phenolic derivatives, polycyclic aromatic hydrocarbons etc.) and inorganic compounds (e.g. heavy metals) which can cause serious disorder. Photocatalytic technology as a part of promising green technology has recently received a lot of interest in contemporary literature for treating pollutants in waste water. ZnO and TiO<sub>2</sub> are well known photocatalysts to degrade organic and inorganic pollutants. However, these materials still require modifications with other nanomaterials because these materials absorb only ultraviolet part of sun light due to wide bandgap and the excitons created under the UV light recombine rapidly. In this talk, I will present our group's recent work about nanostructured TiO<sub>2</sub> based photocatalysts for degradation and detection of organic compounds. Their photocatalytic activity was enhanced through sensitization with carbon/quantum dots, doping with transition metals and functionalization with metal nanoparticles. Enhancement in visible light absorption as well as in charge separation at the interface was obtained through these modifications. These materials are reusable, and their nanostructures do not change after repetitive usage. Our current research focus is to develop visible light activated low-cost and scalable photocatalysts to treat effluent water from industries in particular, pharmaceutical and tannery.

### **Keywords**

Photocatalyst; Dye degradation; Water treatment; Nanofibers; Quantum dots

### **References**

- [1] M. Misra, N. Singh and R. K. Gupta, "Enhanced visible-light-driven photocatalytic activity of Au@Ag core-shell bimetallic nanoparticles immobilized on electrospun TiO<sub>2</sub> nanofibers for degradation of organic compounds" *Catalysis Science & Technology*, 7, 570-580, 2017
- [2] N. Singh, J. Prakash, M. Misra, A. Sharma and R. K. Gupta, "Dual functional Ta doped electrospun TiO<sub>2</sub> nanofibers with enhanced photocatalysis and SERS detection for organic compounds" *ACS Applied Materials & Interfaces*, 9 (34), 28495–28507, 2017
- [3] N. Singh, J. Prakash and R. K. Gupta, "Design and engineering of high-performance photocatalytic systems based on metal oxide-graphene-noble metal nanocomposites" *Molecular Systems Design & Engineering*, 2, 422-439, 2017
- [4] A. Tyagi, K. M. Tripathi, N. Singh, S. Choudhary and R. K. Gupta, "Green synthesis of carbon quantum dots from lemon peel waste: Applications in sensing and photocatalysis" *RSC Advances*, 6, 72423-72432, 2016
- [5] N. Singh, K. Mondal, M. Misra, A. Sharma and R. K. Gupta, "Quantum dot sensitized electrospun mesoporous titanium dioxide hollow nanofibers for photocatalytic applications" *RSC Advances*, 6, 48109 - 48119, 2016

## Session A4

9:00 - 9:30 AM Room A December 18

## A10: Nanoporous gold for sensor and fuel cell catalysts

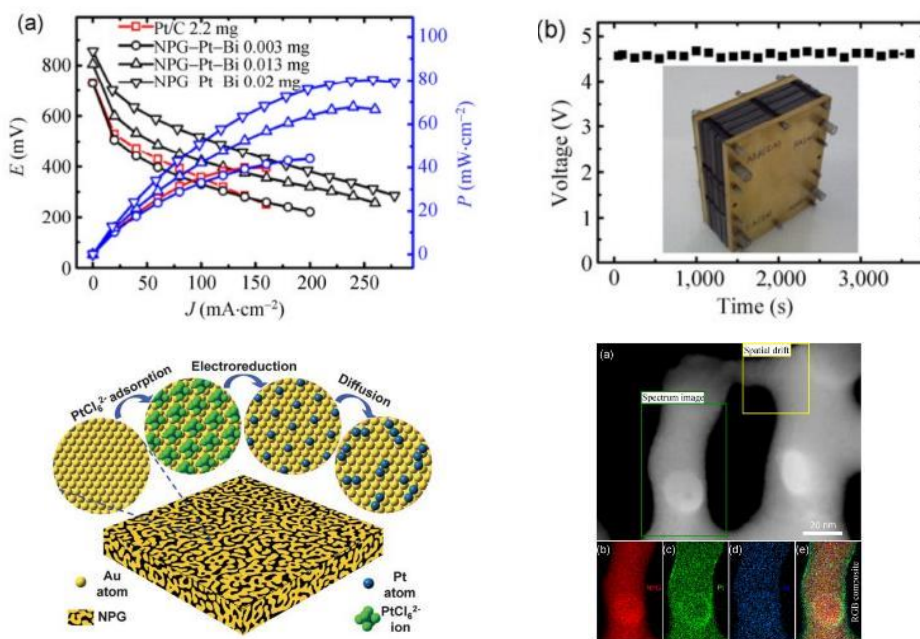
Jianguo Liu\*, Zhigang Zou

College of Engineering and Applied Sciences, Kunshan Innovation Institute, Nanjing University, 22 Hankou Road, Nanjing, Jiangsu Province, China

\*Corresponding author. Email: jianguoliu@nju.edu.cn

**Abstract**

Nanoporous gold (NPG) fabricated by dealloying Au–Ag film in nitric acid shows good performance in the detection of hydrogen peroxide and hydrazine. A maximum power density  $195 \text{ mW cm}^{-2}$  is obtained in a direct hydrazine-hydrogen peroxide fuel cell based on these porous gold leaves. A power density of nearly  $400 \text{ mW cm}^{-2}$  can be observed under the supplying of 10 wt%  $\text{NaBH}_4$  and 20 wt%  $\text{H}_2\text{O}_2$ . When Pt atoms were effectively dispersed onto nanoporous substrate with sub-monolayer precision, the performance of direct formic acid fuel cell in a loading of tens of micrograms is comparable to the one with milligram loading of commercial Pt/C. These NPG–Pt core/shell nanostructures are further decorated by a sub-monolayer of Bi to create highly active reaction sites for formic acid electro-oxidation.



**Fig.** The IV curves, stack, structure of direct formic acid fuel cell using nanoporous gold.

**References**

- [1] *Electrochimica Acta* 56 (2011) 4657–4662
- [2] *Journal of Electroanalytical Chemistry* 661 (2011) 44–48
- [3] *Scientific Reports*, 2012, 2, 941
- [4] *International Journal of Hydrogen Energy*, 2013, 38, 10992-10997
- [5] *Chemical Sciences*, 2014, 5, 403-409
- [6] *Nano Research*, 2014, 7, 1569-1580
- [7] *RSC Advances*, 2017, 7, 18327 - 18332



**Session A4**

**9:30 - 10:00 AM Room A December 18**

**A11: Sensitive Room-Temperature H<sub>2</sub>S Gas Sensors Employing SnO<sub>2</sub> Quantum Wire/Reduced Graphene Oxide Nanocomposites**

Huan Liu\*

*School of Optical and Electronic Information, Huazhong University of Science and Technology, 1037 Luoyu Road, Wuhan, Hubei 430074, China*

\*Corresponding author. Email: huan@mail.hust.edu.cn

**Abstract**

Metal oxide/graphene nanocomposites are emerging as one of the promising candidate materials for developing high-performance gas sensors. Here, we demonstrate sensitive room-temperature H<sub>2</sub>S gas sensors based on SnO<sub>2</sub> quantum wires that are anchored on reduced graphene oxide (rGO) nanosheets. Using a one-step colloidal synthesis strategy, the morphology-related quantum confinement of SnO<sub>2</sub> can be well-controlled by tuning the reaction time, because of the steric hindrance effect of rGO. The as synthesized SnO<sub>2</sub> quantum wire/rGO nanocomposites are spin-coated onto ceramics substrates without further sintering to construct chemiresistive gas sensors. The optimal sensor response toward 50 ppm of H<sub>2</sub>S is 33 in 2 s, and it is fully reversible upon H<sub>2</sub>S release at 22°C. In addition to the excellent gas adsorption of ultrathin SnO<sub>2</sub> quantum wires, the superior sensing performance of SnO<sub>2</sub> quantum wire/rGO nanocomposites can be attributed to the enhanced electron transport resulting from the favorable charge transfer of SnO<sub>2</sub>/rGO interfaces and the superb transport capability of rGO. The easy fabrication and room temperature operation make our sensors highly attractive for ultrasensitive H<sub>2</sub>S gas detection with less power consumption.

**Keywords**

SnO<sub>2</sub> quantum wires; H<sub>2</sub>S; room-temperature; rGO

**Session A4**

**10:00 - 10:30 AM Room A December 18**

**A12: Screened strong light-matter coupling of excitons in multilayer 2D-semiconductors and plasmonic nanocavities**

Jaime Gómez Rivas<sup>1,\*</sup>, Shaojun Wang<sup>1</sup>, Fabio Vaianella<sup>2</sup>, Bjorn Maes<sup>2</sup>, Rasmus H. Godiksen<sup>1</sup>, Alberto G. Curto<sup>1</sup>

<sup>1</sup>*Department of Applied Physics and Institute for Photonic Integration, Eindhoven University of Technology, Eindhoven, The Netherlands*

<sup>2</sup>*Micro and Nanophotonic Materials Group, Faculty of Science, University of Mons, 20 place du Parc, B 7000 Mons, Belgium*

\*Corresponding author. Email: j.gomez.rivas@tue.nl

**Abstract**

Understanding the mechanisms that increase and limit the light-matter coupling strength of excitons in 2D semiconductors to photons in cavities and controlling this coupling is of utmost importance for the development of polaritonic devices. We demonstrate the strong coupling of direct transition excitons in monolayers and multilayers of WS<sub>2</sub> with collective plasmonic resonances in open plasmonic cavities formed by arrays of metallic nanoparticles [1]. The Rabi energy increases by increasing the number of layers. However, this increase does not scale with the square root of the number of layers as expected for strongly coupled systems. Only in-plane coupling contributes to the Rabi energy on the nanoparticle array due to the screened out-of-plane field distribution in WS<sub>2</sub>. The decreased in-plane dipole moments of thicker WS<sub>2</sub> multilayers result in a smaller Rabi energy than the expected value from collective strong coupling.

**Keywords**

Strong light-matter coupling; 2D-semiconductors; Plasmonics; Nanoparticle Arrays; Surface Lattice Resonances

**References**

[1] Shaojun Wang, Quynh Le-Van, Fabio Vaianella, Bjorn Maes, Simone Eizagirre Barker, Rasmus H. Godiksen, Alberto G. Curto, Jaime Gomez Rivas, Screened Strong Coupling of Excitons in Multilayer WS<sub>2</sub> with Collective Plasmonic Resonances, arXiv: 1808.08388

**Session A5**

**11:00 - 11:30 AM Room A December 18**

## **A13: Functional Molecular Junctions derived from Double Self-assembled Monolayers on Graphene**

Sohyeon Seo<sup>2</sup>, Hyoyoung Lee<sup>1,2,\*</sup>

<sup>1</sup>*Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Sungkyunkwan University, Suwon, 16419, Republic of Korea*

<sup>2</sup>*Department of Chemistry, Sungkyunkwan University (SKKU), Suwon 16419, Republic of Korea*

Email: sshyeon@skku.edu (Sohyeon Seo)

### **Abstract**

Information processing through molecular junctions is getting important as the device is miniaturized into a nanoscale. Herein, we report functional molecular junctions derived by double-self-assembled monolayers (SAMs) intercalated between soft graphene electrodes. Newly assembled molecular junctions are fabricated by placing one molecular SAM/(top) electrode on the other molecular SAM/(bottom) electrode *via* a contact-assembly technique. Double-SAMs can provide a tunnelling conjugation across the van der Waals gap between the terminals of each monolayer and exhibit a new electrical function. Robust contact-assembled molecular junctions will be platforms for the development of an equivalent contact molecular junction between top and bottom electrodes, which can be applied independently to different kinds of molecules for either the structural complexity or assembly properties of molecules.

### **Keywords**

molecular junction; double self-assembled monolayer; molecular electronics; graphene electrode; molecular diode

### **Introduction**

Molecular electronics have mainly focused on the well-described charge transport through single molecular junctions or the increase in stability and reproducibility of molecular self-assembled monolayer (SAM) junctions. [1-4] The fascinating points of the bottom-up fabrication using SAMs are its simplicity, low-cost, and reproducibility to at least one contact (*e.g.*, a bottom contact). Thus, the majority of the investigation for bottom-up molecular junctions has been for constructing the homogeneous structures of molecular layers at a top contact as if molecular SAMs are made at a bottom contact.

Here, we suggest new soft-sandwich configurations for solid-state molecular devices (Figure 1). One soft polymer substrate (*e.g.*, polydimethylsiloxane, PDMS) with patterned graphene electrodes can make good contacts through both graphene and PDMS areas on the other one. This can directly form the assembly junction of molecular SAM(s) sandwiched between two graphene/PDMS substrates without the transfer of electrodes such as pressing or flotation. In particular, more complex molecules than alkanethiols that contain large redox centers or functional chains inducing less packing density of SAMs require relevant contacts corresponding to the structures of the SAMs in their molecular junctions. In this work, the molecular SAM-formed top and bottom electrode arrays are vertically positioned to each other and assembled to contact for formation of the crossbar molecular junctions by a simple and reproducible position alignment. Our new equivalent contact-assembly method can provide simple,

stable, reproducible, and length controllable molecular junctions using either one or two kinds of SAM molecules for molecule-based electronics, resulting in new functional molecular junctions derived by double-SAMs.

## Methods

*Materials and characterization:* In order to improve the quality of single-layer graphene, preparation steps such as well drying of a coated polymer film, careful washing of a polymer-coated graphene sheet with floating on water, and well-removing polymer residuals with hot acetone must be carefully conducted. Defect-free or less defective single-layer graphene in high quality is mechanically and chemically very stable. Apparently defect-free or less defective single-layer graphene has been used for the fabrication of graphene electrodes after synthesis; a piece of every CVD graphene batches grown in each CVD tube has been randomly evaluated by optical microscopy, AFM, and Raman after transferring onto a SiO<sub>2</sub> substrate.

*Fabrication of equivalent contact junctions:* Contact-assembled junctions were fabricated by placing one molecular assembled electrode (molecular SAM/graphene) on the other electrode to form a crossbar set of an electrode array. The top and bottom electrodes were softly and equivalently merged onto each other *via* the PDMS//PDMS soft contact, which resulted in stable crossbar junctions in the device.

## Results and Discussion

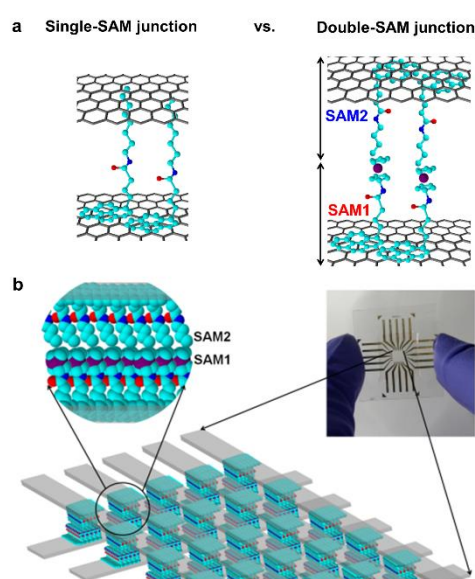
Figure 2a shows histograms of  $\log|J|$  at  $-0.5$  V for the selected data set of  $\log|J|$  within a range of  $\mu \pm 3\sigma$  ( $\mu$  = the average, and  $\sigma$  = the standard deviation) for G<sub>T</sub>/C<sub>n</sub>-C4Pyr/G<sub>B</sub> ( $n = 4, 6, 8, 10$ ). The  $J$  curves (Figure 2b) were plotted on a logarithmic scale as a function of applied voltage for the contact-assembly junctions composed of C<sub>n</sub>-C4Pyr ( $n = 4, 6, 8, 10$ ) SAMs (the error bars represent the standard deviation with 95% confidence intervals on the mean that correspond to the selected  $J$  values from 65-70 junctions). The  $J$  depended exponentially on molecular length (or distance between two electrodes). It is expected that the tunnelling is a dominant mechanism of the charge transport,  $J = J_0 e^{-\beta d}$  (for the rectangular tunnelling barriers, where  $J_0$  is the current density when  $d$  is zero,  $\beta$  is the tunnelling decay constant, and  $d$  is the barrier width) can be applied to the molecular junction.[5-6]

The fit of the  $J$  values from the contact-assembly junctions of C<sub>n</sub>-C4Pyr SAMs was determined at several bias voltages as a function of molecular length. The  $\beta$  values were measured as  $0.69-0.70 \pm 0.01$  Å<sup>-1</sup> in a voltage range from  $-0.1$  to  $-0.5$  V. Considering the effects of defects in bottom electrodes and alkyl SAMs on the value of  $\beta$ , the measured values of  $\beta$  ( $0.5 < \beta < 1.0$ ) can imply low defects corresponding to the results of the voltammetry and the strong interactions between pyrene anchors and graphene electrodes *via* noncovalent  $\pi$ - $\pi$  interactions.

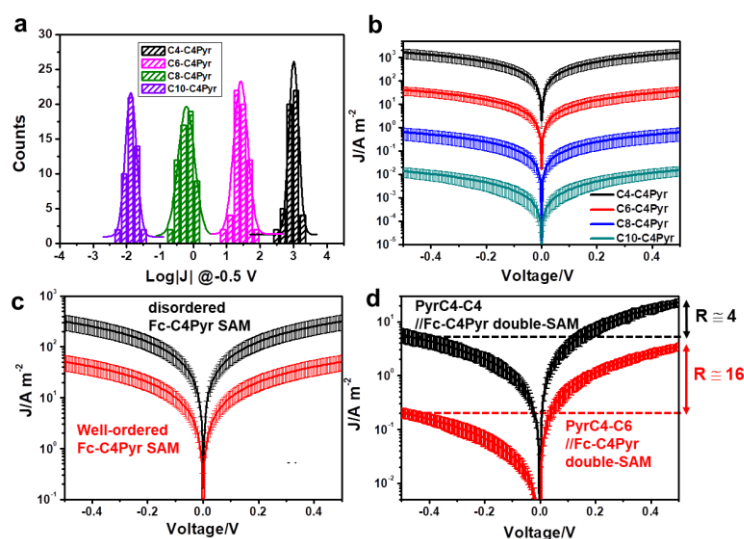
For the functionalized molecular SAM junctions, the charge transport through the Fc-C4Pyr SAMs in our equivalent contact junctions was also measured (Figure 2c). In a voltage range between  $\pm 0.5$  V, we found two different types of  $J$  curves corresponding to two different junction states with regard to the thickness difference of the Fc-C4Pyr SAMs due to the ordering of the large functional groups. The differences in the junction distances in the Fc-C4Pyr SAMs were reflected in their  $J$  curves. The performance of the Fc-C4Pyr SAM showed that the current flow both forward and backward directions acting as an insulating layer as observed with other C<sub>n</sub>-C4Pyr SAM junctions, even though electrochemically active Fc moieties are asymmetrically located near the top electrode. This indicates that the tunnelling barrier between the bottom graphene electrode and the alkyl part is supposed to be similar to that between the Fc unit and the G<sub>T</sub> electrode (including the van der Waals gap), resulting in symmetric potential drops across the Fc part and the alkyl part.

On the other hand, molecular rectifying performance allowing for asymmetrical currents were simply applied using our contact-assembly with the junctions comprised of double-SAMs (*e.g.*, G<sub>T</sub>/PyrC4-C4//Fc-C4Pyr/G<sub>B</sub> or G<sub>T</sub>/PyrC4-C6//Fc-C4Pyr/G<sub>B</sub>, where // denotes a contact between SAMs) (Figure 2d). The  $J$  values measured in the double-SAM junctions (approximately 2.9 nm) of G<sub>T</sub>/PyrC4-C4//Fc-

C4Pyr/G<sub>B</sub> did not follow the tendency of the length-dependent  $J$  plots in Figure 2b, which show relatively higher current densities than that of C10-C4Pyr (approximately 1.8 nm) with a similar molecular length. According to previous papers, the junctions of double-SAMs (e.g., Hg-alkyl SAM1//alkyl SAM2-Hg) exhibited a negligible influence on the van der Waals interface between the two SAMs, and the coupling of the SAM1//SAM2 interfaces was considered to be better than that of the SAM//Hg interfaces. Thus, the molecular length-dependency of the  $J$  values on the double-pyrene SAM junctions might be slightly deviated from the tendency of the single-pyrene SAM junctions on the molecular length-dependent  $J$  values. Although the same pyrene-anchored contacts on both electrodes were formed, this asymmetric double-SAM junction showed significant rectification behaviour in a voltage range of  $\pm 0.5$  V. Furthermore, the rectification ratios in the  $J$  values were increased in junctions of G<sub>T</sub>/PyrC4-C6//Fc-C4Pyr/G<sub>B</sub> in which the distance of the tunnelling barrier increased by the length of the top SAM at a negative bias. Thus, the rectification ratios can be controlled by two different SAMs in the molecular junction assembled by the contacts of two electrodes.



**Figure 1.** (a) Schematics of molecular junctions comprising either single- or double-self-assembled monolayers (SAMs) on graphene. (b) Picture of the device.



**Figure 2.** (a) Histograms of  $\log|J|$  at  $-0.5$  V for the selected data set of  $\log|J|$  within a range of  $\mu \pm 3\sigma$  ( $\mu$  = the average, and  $\sigma$  = the standard deviation) for G<sub>T</sub>/C<sub>n</sub>-C4Pyr/G<sub>B</sub> ( $n = 4, 6, 8, 10$ ). (b) Semi-log plots of  $J$ - $V$  curves of

single SAMs in molecular junctions contact-assembled  $G_T/\text{PyrC4-C}_n$ ,  $n = 4, 6, 8, 10/G_B$ . Pyrene molecular junctions of non-shortened devices that were fabricated with well-patterned graphene electrodes allowed for >90% yield. (c) Semi-log plots of  $J$ - $V$  curves of functionalized single-SAMs in molecular junctions of contact-assembled  $G_T/\text{Fc-C4Pyr}/G_B$ . (d) A new functional  $J$ - $V$  curves (in semi-log plots) of double-SAMs in molecular junctions of contact-assembled  $G_T/\text{PyrC4-C4}/\text{Fc-C4Pyr}/G_B$  and  $G_T/\text{PyrC4-C6}/\text{Fc-C4Pyr}/G_B$ . Rectification ratio values ( $R$ ) are measured by 4 for  $G_T/\text{PyrC4-C4}/\text{Fc-C4Pyr}/G_B$  and 16 for  $G_T/\text{PyrC4-C6}/\text{Fc-C4Pyr}/G_B$ .

## Conclusions

In summary, we showed that newly functionalized molecular junctions using a contact-assembly method that places one molecular SAM/(top) electrode on the other molecular SAM/(bottom) electrode can transduce intermolecular charge transport into electronic signals. On a graphene electrode, pyrene-anchored electrochemically inactive or active molecules were used for noncovalent assembly. The insulating alkyl backbones in  $\text{C}_n\text{-C4Pyr}$  SAM junctions served as a tunnelling distance in a rectangular potential barrier; that is, the current density that flows across the junctions is exponentially dependent on the molecular length at the low bias regime (*e.g.*,  $\pm 0.5$  V). The electrochemically active  $\text{Fc-C4Pyr}$  SAM junctions also showed that the current flow both forward and backward directions at  $\pm 0.5$  V acting as an insulating layer as observed with other  $\text{C}_n\text{-C4Pyr}$  SAM junctions. However, double-SAM junctions of  $G_T/\text{PyrC4-C4}$  (or  $\text{-C6})/\text{Fc-C4Pyr}/G_B$  resulted in the current rectification at  $\pm 0.5$  V in one direction, coming from the asymmetric coupling effects of the HOMO level of the Fc to electrodes. Our new type of robust contact-assembled molecular junctions can be applied to new functional molecular junctions by combining two different molecular SAMs.

## Acknowledgement

This work was supported by IBS-R011-D1.

## References

- [1] M. A. Reed, C. Zhou, C. J. Muller, T. P. Burgin, J. M. Tour, *Science* 1997, 278, 252-254
- [2] H. B. Akkerman, P. W. M. Blom, D. M. de Leeuw, B. de Boer, *Nature* 2006, 441, 69-72
- [3] S. Park, G. Wang, B. Cho, Y. Kim, S. Song, Y. Ji, M.-H. Yoon, T. Lee, *Nat. Nanotechnol.* 2012, 7, 438-442
- [4] Z. Wang, H. Dong, T. Li, R. Hviid, Y. Zou, Z. Wei, X. Fu, E. Wang, Y. Zhen, K. Norgaard, B. W. Laursen, W. Hu, *Nat. Commun.* 2015, 6, 7478
- [5] C. A. Nijhuis, W. F. Reus, G. M. Whitesides, *J. Am. Chem. Soc.* 2010, 132, 18386-18401
- [6] S. Seo, M. Min, S. M. Lee, H. Lee, *Nat. Commun.* 2013, 4, 1920
- [7] P. Song, C. S. S. Sangeeth, D. Thompson, W. Du, K. P. Loh, C. A. Nijhuis, *Adv. Mater.* 2016, 28, 631-639

**Session A5**

**11:30 - 12:00 AM Room A December 18**

**A14: Spin-valley transport property in silicene junction**

Bumned Soodchomshom\*

*Department of physics, Faculty of science, Kasetsart University, Bangkok, Thailand*

\*Corresponding author. Email: Bumned@hotmail.com

**Abstract**

Silicene, a silicon analogue of graphene, is a monolayer of silicon atoms arranged in a honeycomb lattice with large spin orbit coupling and bulked atomic structure. It is a 2-dimensional topological insulator and has attracted increasing attention during the past few years. The carriers in the system governed by the spin-valley dependent massive Dirac fermions. Pseudo mass of Dirac fermions is tunable by external forces such as perpendicular electric field, staggered exchange energy and off resonant circularly polarized light. This may lead to the perfect control of spin-valley polarization in silicene junction. Our talk would give the clarification of how spin-valley filtering in silicene is perfect based on ballistic quantum transport theory.

**Keywords**

Silicene; 2D materials; spin-valley polarization; 2D topological insulator

**Session A5**

**12:00 - 12:30 AM Room A December 18**

**A15: Comparison of electrical energy and power of PV cells or module with different cells materials in clear sky day condition**

Rohit Tripathi<sup>1,2,\*</sup>, T. S. Bhatti<sup>2</sup>, G. N. Tiwari<sup>2</sup>

<sup>1</sup>*School of Electrical, Electronics & Communication Engineering, Galgotias University, G. Noida- U.P., India*

<sup>2</sup>*Centre for Energy Studies, Indian Institute of Technology Delhi, Houz Khas, New Delhi, India*

\*Corresponding author. Email: rohittripathi30.iitd@gmail.com

**Abstract**

In present communication, a comparison has been made on the basis of attainment of the electrical energy and power from solar cells or glass to glass or semitransparent photovoltaic module. To evaluate the electrical energy and power, five different materials or cases have been considered, which are named as: case (i): mono crystalline silicon (c-Si), case (ii): poly crystalline silicon (p-Si), case (iii): amorphous silicon (a-Si), case (iv): cadmium telluride (CdTe) and case (v): *copper-indium-gallium-selenide (CIGS)*. One PV module has been considered for the analysis which dimension is  $0.605 \times 1 \text{ m}^2$ . For case (i): PV cells are made of silicon crystalline, which is having 0.5 Volts and 4 Amp and 36 cells are connected in series, which are producing 72 watts. This analysis has been studied for a clear sky day condition, New Delhi, India. The comparative study is attempted to choose best for generating electrical energy and power due to high electrical demands in our society. It is observed that the maximum electrical energy and power have been obtained for case (i), whereas minimum for case (iii), due to high PV cell temperature. The electrical energy and power have been 1.8 times higher in case (i), than case (iii).

**Keywords**

PV cell; semitransparent module; cell material; power

**References**

- [1] Tripathi R., Tiwari G.N., Al-Helal I.M., "Thermal modeling of N partially covered photovoltaic thermal (PVT)-Compound parabolic concentrator (CPC) collectors connected in series", *Solar Energy*, 123, 2016, 174-184
- [2] Tripathi R., Tiwari G.N., "Annual performance evaluation (energy and exergy) of fully covered concentrated photovoltaic thermal (PVT) water collector: An experimental validation", *Solar energy*, 146, 2017, 180-190
- [3] Cheng C.L., Sanchez Jimenez C.S. Lee M.C., Research of BIPV optimal tilted angle, use of latitude concept for south oriented plans", *Renewable Energy*, 34, 2009, pp. 1644-1650
- [4] Duffie J, Beckman W., *Solar Engineering of Thermal Processes*, Wiley, New York, NY, USA, 1974



**Session A6**

**14:00 - 14:30 PM Room A December 18**

**A16: Printed graphene nanoflakes for radio frequency antennas and wireless sensors**

Xianjun Huang\*, Dongming Zhou, Dongfang Guan

*National University of Defence Technology, NO.109, Deya Road, Changsha, China*

\*Corresponding author. Email: huangxianjun@nudt.edu.cn

**Abstract**

Printed antenna based on graphene nanoflakes has attracted increasing attention from both academic and industrial societies, with its advantages of low cost, high performance, high production efficiency and environmentally friendliness, etc [1-6]. Highly conductive graphene nanoflake laminate can be achieved through graphene nanoflakes dispersion, screen printing and compression laminating. The compression can improve the laminate conductivity by more than 50 times, and improve the radiation efficiency of printed graphene antenna as well [1, 2]. Based on successful demonstration on radiation of printed graphene nanoflakes antenna, more works on printed radio frequency identification (RFID) tag, flexible communication antennas, remote humidity sensors have been developed theoretically and experimentally [1-3, 5]. The results prove that the printed graphene antenna and sensors are the right choices for low-cost, environmentally friendly disposable electronics in internet of things (IoT), smart retails, property management, etc.

**Keywords**

Printed electronics; graphene nanoflakes; flexible antenna; wireless sensing; RFID

**References**

- [1] Huang, X., Leng, T., Zhang, X., Chen, J.C., Chang, K.H., Geim, A.K., Novoselov, K.S. and Hu, Z., Binder-free highly conductive graphene laminate for low cost printed radio frequency applications. *Applied Physics Letters*, 106(20), p.203105 (2015). doi:10.1063/1.4919935
- [2] Huang, X., Leng, T., Zhu, M., Zhang, X., Chen, J., Chang, K., Aqeeli, M., Geim, A.K., Novoselov, K.S. and Hu, Z., Highly flexible and conductive printed graphene for wireless wearable communications applications. *Scientific reports*, 5, p.18298 (2015). doi:10.1038/srep18298
- [3] Leng, T., Huang, X., Chang, K., Chen, J., Abdalla, M.A. and Hu, Z., Graphene nanoflakes printed flexible meandered-line dipole antenna on paper substrate for low-cost RFID and sensing applications. *IEEE Antennas and Wireless Propagation Letters*, 15, pp.1565-1568 (2016). doi:10.1109/LAWP.2016.2518746
- [4] Huang, X., Leng, T., Chang, K.H., Chen, J.C., Novoselov, K.S. and Hu, Z., Graphene radio frequency and microwave passive components for low cost wearable electronics. *2D Materials*, 3(2), p.025021 (2016).
- [5] Huang, X., Leng, T., Georgiou, T., Abraham, J., Nair, R.R., Novoselov, K.S. and Hu, Z., Graphene oxide dielectric permittivity at GHz and its applications for wireless humidity sensing. *Scientific reports*, 8(1), p.43 (2018). doi:10.1038/s41598-017-16886-1
- [6] Akbari, M., Khan, M.W.A., Hasani, M., Bjorninen, T., Sydanheimo, L. and Ukkonen, L., Fabrication and characterization of graphene antenna for low-cost and environmentally friendly RFID tags. *IEEE Antennas Wirel. Propag. Lett*, 15, pp.1569-1572 (2015). dos:10.1109/LAWP.2015.2498944

**Session A6**

**14:30 - 15:00 PM Room A December 18**

**A17: Bio-inspired on-surface fabrication of graphene nanoribbons**

Hiroshi Sakaguchi\*

*Institute of Advanced Energy, Kyoto University: Uji, Kyoto, 611-0031, Japan*

\*Corresponding author. Email: sakaguchi@iae.kyoto-u.ac.jp

**Abstract**

Heterogeneous catalysis has been known to produce functional materials by the acceleration of chemical reactions on metal surface. In conventional heterogeneous catalysis, the reaction can be accelerated by electronic interactions between the reactant and metal surface, like a “hard (scrap & built)” manner. In this study, we demonstrate a synthesis of graphene nanoribbons (GNRs) by a new concept of “bio-inspired heterogeneous catalysis” similar to the enzymatic reactions in biology like a “soft” manner, which is featured by homo chirality, transformation, self-assembly and adaptation, directing an optimized chemical reaction pathway to efficiently produce the product. Our developed two-zone chemical vapor deposition of the “Z-bar-linkage” precursors designed herein, exhibiting flexible as well as complex geometry that allows them to adopt chiral (asymmetrical) conformations on a Au(111) surface, results in the efficient formation of acene-type graphene nanoribbons with a width of 1.45 nm through optimized cascade reactions. These new surface-reactions include the formation of self-assembled homochiral polymers in a chain with a planar conformation, followed by efficient stepwise dehydrogenation via a conformation-controlled mechanism. The FET devices of acene-type GNR transferred from Au(111) to the insulating substrates show an excellent semiconductor performance. Thus, our proposed concept of “bio-inspired heterogeneous catalysis” is useful to fabricate the new nanocarbon materials.

**Keywords**

Graphene nanoribbons; Surface Science

**References**

- [1] H. Sakauchi; et al., Homochiral Polymerization-driven Selective Growth of Graphene Nanoribbons. *Nature Chemistry*, 9, 57 (2017). doi:10.1038/nchem.2614
- [2] H. Sakauchi; et al., Width-Controlled Sub-Nanometer Graphene Nanoribbon Films Synthesized by Radical-Polymerized Chemical Vapor Deposition. *Advanced Materials*, 26, 4134 (2014). doi:10.1002/adma.201305034
- [3] H. Sakauchi; et al., Strain-induced Skeletal Rearrangement of a Polycyclic Aromatic Hydrocarbon on a Copper Surface. *Nature Communications*, 8, 16089 (2017). doi:10.1038/ncomms16089

## Session A6

15:00 - 15:30 PM Room A December 18

## A18: Facile Synthesis of 2D Nitrogen-Containing Porous Carbon Nanosheets Induced by Graphene Oxide for High-Performance Supercapacitors

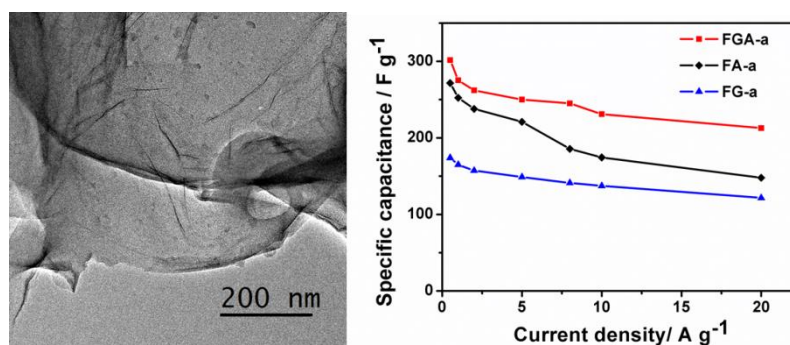
Xu Zhang\*, Qiuyu Fan, He Yang, Ning Qu, Yonghou Xiao

State Key Laboratory of Fine Chemicals, School of Petroleum and Chemical Engineering, Dalian University of Technology, Panjin 124221, China

\*Corresponding author. Email: zhangxu@dlut.edu.cn

**Abstract**

Two-dimensional (2D) nitrogen-containing porous carbon nanosheets are the ideal electrode materials for supercapacitors, which also have been the focus of increasing attention in recent years [1]. 2D nitrogen-containing porous carbon nanosheets are prepared in the presence of graphene oxide (GO) as a structure-directing agent by a simple yet facile hydrothermal method. It is found that GO can effectively turn the morphologies of the hydrothermal carbonaceous products, resulting in the unique 2D structures. The as-obtained 2D nitrogen-containing porous carbon nanosheets as electrodes for supercapacitors exhibit a high specific capacitance of  $301.6 \text{ F g}^{-1}$  at a current density of  $0.5 \text{ A g}^{-1}$  and superior rate capability with a capacitance retention of 70.5% at the high current density of  $20 \text{ A g}^{-1}$ . The 2D nitrogen-containing porous carbon nanosheet electrodes also exhibit good cycling performance, possessing the high capacitance retention over 92.3 % after 5000 charge-discharge cycles at the current density of  $5 \text{ A g}^{-1}$ . Such superior electrochemical performance of the 2D nitrogen-containing porous carbon nanosheets could be attributed to the high pseudocapacitive effect of the nitrogen-containing species and the peculiar structural characteristics featuring the short ion transport distance and abundant porous channels.



**Fig.** TEM image and the electrochemical performance of 2D carbon nanosheets

**References**

[1] R. Ma and T. Sasaki, *Accounts Chem. Res.*, 2015, 48, 136

**Session A7**

**16:00 - 16:30 PM Room A December 18**

## **A19: Electrochemical Synthesis of Nano-Structured Si for Energy Storage Application**

Anjali Vanpariya, Manmohansingh Waldiya, Dharini Bhagat, Harsh Chaliyawala, Sakshum Khanna, Roma Patel, Nisarg shah, Indrajit Mukhopadhyay\*

*Department of Solar Energy, Pandit Deendayal Petroleum University, Raysan Gujarat, India*

\*Corresponding author. Email: Indrajit.M@sse.pdpu.ac.in

### **Abstract**

In this paper we have systematically investigated the electrodeposition of silicon over highly conductive substrates. Crystalline silicon was effectively electrodeposited on gold (Au (111)) and graphene coated copper substrates in the over potential regime using  $\text{SiCl}_4$  in water contaminated 1-Butyl-3-Methylimidazolium-Bis (Trifluoromethylsulfonyl) imide (BMImTf<sub>2</sub>N) under ambient conditions. It was observed that the existence of water in the ionic liquid (BMImTf<sub>2</sub>N) does not affect the effective potential window significantly but it tends to induce template effect that lead to the deposition of inter-connected spherical Si particle. However, active electrolyte in water contaminated ionic liquid has been found to react with the copper substrate, forming a semiconductor film of copper oxide. In order to eliminate the oxide formation, graphene sheets were coated over copper substrates and were further used to deposited silicon. Initially, graphene (RGO) coated copper substrate was prepared from reduction of graphene oxide in Ar/H<sub>2</sub> containing atmosphere at high temperature before electrodeposition. The three-dimensional growths of nanospheres were characterized using scanning and transmission electron microscopy and X-ray photoelectron spectroscopy. The key findings of the obtained results was the formation of silicon nanospheres from the precursor ( $\text{SiCl}_4$ ) which coexisted with ionic liquids and not undergoing hydrolysis even in the presence of water. In the present talk, the key to the formation of various Si morphologies on the substrate of different surface energy will be discussed on the basis of nucleation and growth mechanism from the current time relationship. Initial findings on the application of inter-connected Si nano-spheres on Au(111) in supercapacitors will also be presented.

**Session A7**

**16:30 - 17:00 PM Room A December 18**

## A20: Coherent phonons of high- and low-symmetry in the topological insulators

Oleg V. Misochko\*

*Institute of Solid State Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow region, Russia*

\*Corresponding author. Email: misochko@issp.ac.ru

### Abstract

Coherent and incoherent Raman active phonons in the 3D topological insulators, Bi<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Se<sub>3</sub>, have been studied with ultrafast laser and spontaneous Raman spectroscopy [1-4]. The differences between coherent and incoherent phonons are revealed through a comparison of spontaneous Raman spectra and Fourier transforms of time-resolved reflectivity [2]. Polarization dependence and different detection schemes (isotropic and anisotropic) allow to separate fully symmetric A<sub>1g</sub> and doubly degenerate E<sub>g</sub> phonons in the time-domain experiments [2]. Using coherent control to selectively excite a single fully symmetric mode [4] we observe its coupling to surface Dirac plasmon. The coupling results in a short-lived frequency chirp of the coherent A<sub>1g</sub> phonon and the transient coherent phonon spectra obtained at different time frames exhibiting a Fano-like asymmetric lineshape attributed to a quantum interference between continuum-like coherent Dirac plasmons and phonons [5]. By analyzing the chirp lifetime and the time-dependent asymmetric line shape, it was established that the Fano-like resonance persists up to several hundred femtoseconds.

### Keywords

Ultrafast spectroscopy; Coherent phonons; Topological insulators; Time- and frequency-domain; 3D Dirac plasmons

### References

- [1] K. Norimatsu, M. Hada, S. Yamamoto, T. Sasagawa, M. Kitajima, Y. Kayanuma, and K. G. Nakamura. *J. Appl. Phys.* 117, 143102 (2015). doi: 10.1063/1.4917384
- [2] O.V. Misochko, M.V. Lebedev, *JETP* 126, 64 (2018). doi: 10.1134/S106377611801017X
- [3] O.V. Misochko, J. Flock, and T. Dekorsy, *Phys. Rev. B* 91, 174303 (2015). doi: 10.1103/PhysRevB.91.174303
- [4] J. Hu, K. Igarashi, T. Sasagawa, K.G. Nakamura, and O.V. Misochko, *J. Appl. Phys.* 112, 031901 (2018). doi: 10.1063/1.5016941
- [5] R. Mondal, A. Arai, Y. Saito, P. Fons, A.V. Kolobov, J. Tominaga, and M. Hase, *Phys. Rev. B* 97, 144306 (2018). doi:10.1103/PhysRevB.97.144306

**Session A7**

**17:00 - 17:30 PM Room A December 18**

**A21: Switchable valley polarization by external electric field effect in graphene/CrI<sub>3</sub> heterostructures**

M. Umar Farooq, Jisang Hong\*

*Affiliation Information: Department of Physics, Pukyong National University, Busan 608-737, Republic of Korea*

\*Corresponding author. Email: hongj@pknu.ac.kr

**Abstract**

Achieving and controlling the valley polarization is a core issue for valleytronics applications. Conventionally, the valley polarization was achieved by applying the external magnetic field or structural manipulation. However, this approach is less efficient. Here, we explored the single layer and bilayer graphene on CrI<sub>3</sub> (g-CrI<sub>3</sub> and 2g-CrI<sub>3</sub>) heterostructures to induce the valley polarization. In g-CrI<sub>3</sub>, we found a huge valley polarization with the majority gap difference of  $\Delta_{1\uparrow} - \Delta_{2\uparrow} = 44$  meV. Even in 2g-CrI<sub>3</sub> system, we also found the valley polarization of  $\Delta_{1\uparrow} - \Delta_{2\uparrow} = 21$  meV. Moreover, we also investigated the electric field effect on the valley polarization. In both systems, we obtained that the valley polarisation could be switched in the majority spin band. For instance, the sign of gap difference at  $\pm K$  changed from  $\Delta_{1\uparrow} > \Delta_{2\uparrow}$  at zero field to  $\Delta_{1\uparrow} < \Delta_{2\uparrow}$  at a small applied electric field of 0.1 V/Å. With further increase of the electric field to 0.2 V/Å, the valley polarisation disappeared. Thus, we propose that a large value of valley polarisation can be achieved and the sign of polarization can also be switched with electric field instead of magnetic field. This feature will be very beneficial for designing of valleytronic based information process devices.

**Keywords**

Heterostructures; Valley polarization; Valleytronics; Switchable valley polarization; pseudospin

**Session B4**

**9:00 - 9:30 AM Room B December 18**

## **B11: Metasurfaces for Solar Thermophotovoltaic Energy Harvesting**

Abul K. Azad<sup>1,\*</sup>, Chun-Chieh Chang<sup>1</sup>, Wilton J. M. Kort-Kamp<sup>2</sup>, Milan Sykora<sup>3</sup>, Diego A. R. Dalvit<sup>2</sup>, Hou-Tong Chen<sup>1</sup>

<sup>1</sup>Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

<sup>2</sup>Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

<sup>3</sup>Chemistry Division, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

\*Corresponding author. Email: aazad@lanl.gov

### **Abstract**

Solar energy promises a viable solution to meet the ever-increasing power demand by providing a clean, renewable energy alternative to fossil fuels. Photovoltaic (PV) solar cells have been the most prevalent solar energy harvesting technology. Despite the development over the past few decades, the efficiency of state-of-the-art, single-junction PV cells is still far below the fundamental limit predicted by Shockley and Queisser. Metasurface inspired solar thermophotovoltaics (STPV) [1] represent a promising alternative to traditional photovoltaics for solar energy harvesting. We demonstrate a broadband, polarization independent, omnidirectional absorber based on a metallic metasurface architecture, which accomplishes greater than 90% absorptance in the visible and near-infrared range of the solar spectrum, and exhibits low emissivity at mid- and far-infrared wavelengths [2]. While the gold metasurface exhibits high absorptance its application for the high temperature STPV is not possible because of the inherent low melting temperature of gold. We also demonstrate refractory metasurfaces for STPV with tailored absorptance and emittance characterized by in-situ high-temperature measurements, featuring thermal stability up to at least 1200 °C. Our tungsten-based metasurface absorbers have close-to-unity absorption from visible to near infrared and strongly suppressed emission at longer wavelengths, while our metasurface emitters provide wavelength-selective emission spectrally matched to the band-edge of InGaAsSb photovoltaic cells [3]. The projected overall STPV efficiency is as high as 18% when employing a fully integrated absorber/emitter metasurface structure, much higher than those achievable by stand-alone PV cells.

### **Keywords**

Metasurfaces; refractory metamaterials; solar thermophotovoltaics; solar absorbers; thermal emitters; high-temperature

### **References**

- [1] P. A. Davies, A. Luque, Sol. Energy Mater. Sol. Cells 33, 11 (1994)
- [2] Abul. K Azad, W. JM Kort-Kamp, M. Sykora, N. Weisse-Bernstein, T. S Luk, A. J Taylor, D. A. R Dalvit, and H-T Chen, Scientific Reports 6, 20347 (2016)
- [3] C.-C. Chang, W. J. M. Kort-Kamp, J. Nogan, T. S. Luk, A. K. Azad, A. J. Taylor, D. A. R. Dalvit, M. Sykora, and H.-T. Chen, Nano Letters (2018) (submitted)

**Session B4**

**9:30 - 10:00 AM Room B December 18**

**B12: Solar cell and photoelectrochemical properties of  $\text{Cu}_2\text{ZnSnS}_4$  thin films fabricated by wet chemical techniques**

Shigeru Ikeda<sup>1\*</sup>, Feng Jiang<sup>2</sup>, Thi Hiep Nguyen<sup>3</sup>, Takashi Harada<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science and Engineering, Konan University: 8-9-1 Okamoto, Higashinada, Kobe 658-8501, Japan

<sup>2</sup>Institute of Optoelectronic Materials and Technology, South China Normal University, No.55, Zhongshan Avenue West, Guangzhou, Guangzhou 510631, China

<sup>3</sup>Research Center of Solar Energy Chemistry, Osaka University, 1-3 Machikaneyama, Toyonaka, 560-8531, Japan

\*Corresponding author. Email: s-ikeda@konan-u.ac.jp

**Abstract**

Kesterite compounds of  $\text{Cu}_2\text{ZnSnS}_4$  (CZTS) has been studied for low-cost thin film solar cells because they do not contain toxic and/or rare elements which are included in commercial photo-absorbers of CdTe and  $\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ . The CZTS compound is also attractive for the solar cell because of its optimum band gap energies for sunlight absorption (1.5 eV) and high absorption coefficient ( $> 10^4 \text{ cm}^{-1}$ ). For fabrication of its thin film form, non-vacuum technologies are preferable in view of cost effectiveness. In this study, CZTS thin films with various compositions and additives were fabricated by electrodeposition and spray pyrolysis methods; their solar cell properties and applications for photoelectrochemical sunlight conversion, e.g., water splitting, were also studied [1-8].

**Keywords**

Kesterite  $\text{Cu}_2\text{ZnSnS}_4$ , sputter deposition, solar cell properties, photoelectrochemical water splitting

**References**

- [1] F. Jiang; S. Ikeda; T. Harada; M. Matsumura, *Adv. Energy Mater.*, 4, 1301381 (2014). doi: 10.1002/aenm.201301381
- [2] T. H. Nguyen; W. Septina; S. Fujikawa; F. Jiang; T. Harada; S. Ikeda, *RSC Adv.*, 5, 77565 (2015). doi: 10.1039/C5RA13000J
- [3] F. Jiang; C. Ozaki; Gunawan; T. Harada; Z. Tang; T. Minemoto; Y. Nose; S. Ikeda, *Chem. Mater.*, 28, 3283 (2016). doi: 10.1021/acs.chemmater.5b04984
- [4] T. H. Nguyen; T. Harada; J. Chantana; T. Minemoto; S. Nakanishi; S. Ikeda, *ChemSusChem*, 9, 2414 (2016). doi: 10.1002/cssc.201600641
- [5] T. H. Nguyen; T. Kawaguchi; J. Chantana; T. Minemoto; T. Harada, S. Nakanishi; S. Ikeda, *ACS Appl. Mater. Interfaces*, 10, 5455 (2018). doi:10.1021/acsami.7b14929
- [6] F. Jiang; Gunawan; T. Harada; Y. Kuang; T. Minegishi; K. Domen; S. Ikeda, *J. Am. Chem. Soc.*, 137, 13691 (2015). doi: 10.1021/jacs.5b09015
- [7] F. Jiang; S. Li, C. Ozaki; T. Harada; S. Ikeda, *Sol. RRL*, 2, 1700205 (2018) doi: 10.1002/solr.201700205
- [8] D. Huang; K. Wang; L. Yu; T. H. Nguyen; S. Ikeda; F. Jiang, *ACS Energy Lett.*, 3, 1875 (2018). doi: 10.1021/acsenergylett.8b01005



**Session B4**

**10:00 - 10:30 AM Room B December 18**

**B13: A novel absorber material ZnSnP<sub>2</sub> – crystal growth and device**

Yoshitaro NOSE\*, Shigeru NAKATSUKA, Taro KUWANO, Ryoji KATSUBE

*Department of Materials Science and Engineering, Kyoto University: Yoshida- Honmachi, Sakyo-ku, Kyoto 606-8501, Japan*

\*Corresponding author. Email: nose.yoshitaro.5e@kyoto-u.ac.jp

**Abstract**

Compound semiconductor, ZnSnP<sub>2</sub> is a promising material for absorber in photovoltaic devices due to the absorption coefficient of about 10<sup>5</sup> cm<sup>-1</sup> in the visible light region and the bandgap of 1.6 -1.7 eV, which leads to the theoretical conversion efficiency of about 30 % calculated based on Shockley-Queisser limit. Moreover, ZnSnP<sub>2</sub> consists of earth-abundant and less toxic elements compared to GaAs and CdTe.

In this talk, our recent progress on ZnSnP<sub>2</sub> solar cells will be presented. As you know, thin films are used for absorption layers in solar cells of compound semiconductors because their absorption coefficients are generally high. However, the fabrication processing of ZnSnP<sub>2</sub> thin films have not completely established yet. In our work, bulk crystals of ZnSnP<sub>2</sub> were thus utilized similar to recent studies on CdTe solar cells. [1] The bulk crystals were obtained by solution growth according to the experimentally-established phase diagram [2]. The properties of ZnSnP<sub>2</sub> bulk crystals, such as hole density and mobility, were suitable for absorber in solar cells. Another topic is the structural control of the interface between ZnSnP<sub>2</sub> and back contact. In general, Mo is used for a contact material. In the case of ZnSnP<sub>2</sub> solar cells, the contact of Mo and ZnSnP<sub>2</sub> showed high resistance and while Cu/ZnSnP<sub>2</sub> contact heat-treated led to ohmic behavior [3]. The cross-sectional TEM observation of Cu/ZnSnP<sub>2</sub> interface revealed the formation of Cu<sub>3</sub>P due to interdiffusion at the interface. The results indicate that Cu<sub>3</sub>P contributed to low resistance. The interface between buffer materials and ZnSnP<sub>2</sub> was also investigated using XPS measurements, which clarified that ZnS and In<sub>2</sub>S<sub>3</sub> were favorable compared to CdS from the viewpoint of conduction band offset [4]. The present best efficiency is 3.44 % for ZnSnP<sub>2</sub> solar cells with the structure of Al/AZO/ZnO/(Cd,Zn)S/ZnSnP<sub>2</sub>/Cu [5].

**Keywords**

chalcopyrite phosphide, bulk crystals, heterointerface, lattice mismatch, band alignment

**References**

- [1] J. M. Burst et al., CdTe solar cells with open-circuit voltage breaking the 1 V barrier, *Nature Energy* 1, 16015 (2016). doi:10.1038/nenergy.2016.15
- [2] S. Nakatsuka et al., Bulk crystal growth and characterization of ZnSnP<sub>2</sub> compound semiconductor by flux method, *Phys. Status Solidi (c)*, 12, 520 (2015). doi: 10.1002/pssc.201400291
- [3] S. Nakatsuka et al., Impact of hetero-interfaces in solar cells using ZnSnP<sub>2</sub> bulk crystals, *ACS Appl. Mater. Interface*, 9 33827 (2017). doi: 10.1021/acsami.7b08852
- [4] S. Nakatsuka et al., Band offset at the heterojunction interfaces of CdS/ZnSnP<sub>2</sub>, ZnS/ZnSnP<sub>2</sub> and In<sub>2</sub>S<sub>3</sub>/ZnSnP<sub>2</sub>, *J. Appl. Phys.*, 119, 193107 (2016). doi: 10.1063/1.4950882
- [5] S. Akari et al., ZnSnP<sub>2</sub> solar cell with (Cd,Zn)S buffer layer: Analysis of recombination rates, *Sol. Energy Mater. Sol. Cells*, 174, 412 (2018). doi: 10.1016/j.solmat.2017.09.035

**Session B5**

**11:00 - 11:30 AM Room B December 18**

## **B14: Solar energy conversion to high-value-added reagents on nanoporous sponge photoanodes**

Tomohiko NAKAJIMA\*, Tetsuo TSUCHIYA, Kazuhiro SAYAMA

*National Institute of Advanced Industrial Science and Technology, Tsukuba Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan*

\*Corresponding author. Email: t-nakajima@aist.go.jp

### **Abstract**

Solar hydrogen production from water is an important goal for energy production; however, the current solar-to-hydrogen (STH) efficiency is still not commercially feasible. The STH efficiency should stably exceed 10–20%. Thus, we have been searching for other applications of photoelectrodes driven by sunlight. Solar hydrogen production in Photoelectrochemical (PEC) systems is a cathode reaction, and oxygen gas is obtained at the photoanodes. Oxygen gas has a market value less than several tens of percent that of hydrogen gas; therefore, few studies have focused on the other products except oxygen at photoanodes. Mi *et al.* and Sayama reported that some products, such as peroxydisulfate ( $S_2O_8^{2-}$ ),  $Ce^{4+}$ ,  $IO_4^-$ , and  $H_2O_2$  in the  $WO_3$  photoanode system [1,2]. These reagents have a much higher market value than oxygen. In this work, we focused on the availability of these high-value-added anode products obtained by PEC solar hydrogen production.

We prepared  $WO_3$  nanosponge photoanodes by a nanoparticle/solution hybrid dispersion-deposition. The  $WO_3$  nanosponge photoanodes showed a large photocurrent ( $3.04 \text{ mA}\cdot\text{cm}^{-2}$ ) in 1.0 M  $H_2SO_4$  electrolyte under 1-Sun illumination. This high photocurrent arose from the robust inter-nanoparticle connections and preservation of the nanopores in the photoanode. The absorbed photon-to-current efficiency spectra showed a high maximum of 95.4% at 410 nm. The Faraday efficiency of  $S_2O_8^{2-}$  and  $H_2$  evolution was almost 100%, and the applied bias photon-to-current efficiency for  $S_2O_8^{2-}$  and  $H_2$  was calculated to be 2.45%, which is the highest reported value [3]. We also report a new sustainable chromic acid oxidation process ( $Cr^{6+}$  ion recycling system) for other useful organic reagents production by using this efficient  $WO_3$  nanosponge photoanodes [4]. Obtaining this kind of high-value-added product efficiently at photoanodes in photoelectrochemical systems is important for the use of sunlight in sustainable industrial chemistry.

### **Keywords**

Solar energy; Solar hydrogen; Photoelectrode;  $WO_3$ ; Nanostructure; Photoelectrochemical reaction

### **References**

- [1] Q. Mi et al., *Energy Environ. Sci.*, 2012, 5, 5694
- [2] K. Sayama, *ACS Energy Lett.*, 2018, 5, 5694
- [3] T. Nakajima et al., *J. Mater. Chem. A*, 2016, 4, 17809
- [4] T. Nakajima et al., *J. Mater. Chem. A*, 2018, 6, 110

**Session B5**

**11:30 - 12:00 PM Room B December 18**

**B15: Key technologies for the novel solar driven heating and cooling systems**

Xudong Zhao\*

*University of Hull, United Kingdom*

\*Corresponding author. Email: xudong.zhao@hull.ac.uk

**Abstract**

The paper addressed several key technologies that enable solar driven heating and cooling systems for buildings to operate in efficient and effective ways. In terms of the solar heating, the multiple-throughout-flowing featured panels-array in combination with micro-channel structure for individual panels are the most creative technologies that has proven to be able to achieve 10% higher solar thermal efficiency and 100% higher energy efficiency ratio compared to the existing solar thermal system. In addition, the coupled heat storage/exchanger with the double containers is able to speed up heating time and increase the heat transfer capacity of the system, and is regarded as an additional initiative. The cost balance approach is applied to determine the quantity and area of the PV panel, leading to a new way of achieving the zero-bill heating operation in an economic way. In terms of the solar cooling, the innovative super-performance dew point cooling involving advanced fibre materials, superior thermal-assisted pressing approach for bonding of the fibre material with dry side material, as well as intelligent control of the pump and fan is detailed. Furthermore, the solar driven adsorbent bed cyclic system using the solar radiation and solar based microwave energy was introduced.

**Keywords**

Solar; heating; cooling; multiple-throughout-flowing; micro-channel; double-container; combined heat storage/exchanger; cost-balance approach; dew-point-cooling; adsorbent bed cycling; microwave

**Recent Publications**

- [1] Peng Xu, Xiaoli Ma\*, Xudong Zhao\*, Kevin Fancey. Experimental investigation of a super performance dew point air cooler. *Applied Energy* 203 (2017) 761–777.
- [2] T. M.O. Diallo, X. Zhao\*, A. Dugue, P. Bonnamy, F. J. Miguel, A. Martinez, T. Theodosiou, J. Liu, N. Brown. Numerical investigation of the energy performance of a ventilated façade system employing a smart modular heat recovery unit and a latent heat thermal energy system. *Applied Energy* 205 (2017) 130-152.
- [3] Jinzhi Zhou, Xudong Zhao\*, Xiaoli Ma, Zhenyu Du, Yi Fan, Yuanda Chen, Xinghui Zhang. Clear-days operational performance of a hybrid experimental space heating system employing the novel mini-channel solar thermal & PV/T panels and a heat pump. *Solar Energy* 155 (2017) 464–477.
- [4] Wansheng Yang, Hao Deng, Zhangyuan Wang \*, Xudong Zhao, Song He. Performance investigation of the novel solar-powered dehumidification window for residential buildings. *Energies* 2017, 10, 1369; doi:10.3390/en10091369.
- [5] Zhiyin Duan, Xudong Zhao, Junming Li. Design, fabrication and performance evaluation of a compact regenerative evaporative cooler: Towards low energy cooling for buildings. *Energy* 140 (2017) 506 – 519.

**Session B6**

**14:00 - 14:30 PM Room B December 18**

**B16: Silicon Photonics for 2020 and beyond**

Zhoufeng Ying<sup>1</sup>, Chenghao Feng<sup>1</sup>, Zheng Zhao<sup>1</sup>, David Z. Pan<sup>1</sup>, Ray T. Chen<sup>1,2,\*</sup>

<sup>1</sup>*Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas 78712, USA*

<sup>2</sup>*Omega Optics, Inc., 8500 Shoal Creek Blvd., Bldg. 4, Suite 200, Austin, TX 78757, USA*

\*Corresponding author. Email: chenrt@austin.utexas.edu

**Abstract**

Silicon photonics is poised to revolutionize inter- and intra-data center communications since internet traffic continues to increase exponentially making it difficult and costly for existing switching and interconnects in data centers to cope with the fast-growing bandwidth requirement. Silicon photonics is able to contribute data centers in terms of the lower cost, higher bandwidth, and lower power consumption. As many fundamental components including the power-efficient modulators mature, silicon photonics is believed to have reached the tipping point with a surging global market. Besides the optical interconnects, silicon photonics also shows the promise in abundant applications, ranging from high performance computing and autonomous cars, to biomedical sensing and even aerospace applications.

In this invited speech, an overview of the silicon photonics as well as a potential trend for 2020 and beyond will be provided. First, the recent development of optical components including passive and active modules as well as optical circuits in silicon photonics will be presented. [1] Second, as Moore's law has been approaching the physical limitation, photonics-based high-performance computing is envisioned as a potential answer to the continuation of Moore's law. We propose and experimentally demonstrate a new photonics-assisted full adder which is capable of operating at a higher frequency than electrical counterparts while consuming less power. [2–4] This paves the way to the future integrated high-speed and power-efficient optical computing. Sensing related applications will also be addressed in the presentation. Finally, the main challenges that require technical breakthroughs for the upcoming years will be discussed.

**Keywords**

Silicon photonics; integrated photonics; optical interconnect; optical computing

**References**

- [1] H. Subbaraman, X. Xu, A. Hosseini, X. Zhang, Y. Zhang, D. Kwong, and R. T. Chen, "Recent advances in silicon-based passive and active optical interconnects," *Opt. Express* 23, 2487–2510 (2015)
- [2] Z. Ying, Z. Wang, Z. Zhao, S. Dhar, D. Z. Pan, R. Soref, and R. T. Chen, "Silicon microdisk-based full adders for optical computing," *Opt. Lett.* 43, 983–986 (2018)
- [3] Z. Ying, S. Dhar, Z. Zhao, C. Feng, R. Mital, C.-J. Chung, D. Z. Pan, R. A. Soref, and R. T. Chen, "Electro-optic ripple-carry adder in integrated silicon photonics for optical computing," *IEEE J. Sel. Top. Quantum Electron.* 24, 1–10 (2018)
- [4] Z. Ying, Z. Zhao, C. Feng, R. Mital, S. Dhar, D. Z. Pan, R. Soref, and R. T. Chen, "Automated logic synthesis for electro-optic logic-based integrated optical computing," *Opt. Express* 26, 28002–28012 (2018)

**Session B6**

**14:30 - 15:00 PM Room B December 18**

**B17: Light emission effects mediated by Bloch Surface Waves**

Emiliano Descrovi<sup>1,\*</sup>, Ugo Stella<sup>1</sup>, Natascia De Leo<sup>2</sup>, Luca Boarino<sup>2</sup>

<sup>1</sup>*Department of Applied Science and Technology, Politecnico di Torino, C.so Duca degli Abruzzi 24, Torino, IT-10129, Italy*

<sup>2</sup>*Quantum Research Labs & Nanofacility Piemonte, Nanoscience & Materials Division, Istituto Nazionale di Ricerca Metrologica, Strada delle Cacce 91, Torino, IT-10135, Italy*

\*Corresponding author. Email: emiliano.descrovi@polito.it

**Abstract**

The management of spontaneous light emission at the nanoscale is a crucial aspect in many application domains dealing with lighting, optical communications and quantum information systems. Two widespread approaches to address this issue are based on plasmonic structures and dielectric photonic crystals, which have demonstrated a high potential in controlling spectral, angular and temporal features of the emission. Both approaches exhibit rather complementary advantages, and many efforts are nowadays undertaken to target hybrid solutions taking the best from the two sides.

In this framework, we propose a photonic device based on a dielectric multilayer, which is shown to control the spontaneous emission from organic emitters deposited on its surface [1]. Such a result is achieved by exploiting a near-field interaction of emitters to Bloch Surface Waves [2, 3] resonantly coupled within a circular cavity surrounded by a diffractive structure. A bright, monochromatic emission is then obtained, with spectral width below 1 nm, a spontaneous decay rate enhanced by a factor varying from 15 to 30, and a propagation divergence below 5 degrees in free space [4]. These findings are particularly promising for application in the technological field of integrated light sources operating in a single-photon regime.

**Keywords**

Surface Waves; Photonic Nano Cavity; Purcell effect; Directional Emission

**References**

- [1] M. Ballarini; F. Frascella; F. Michelotti; G. Digregorio; P. Rivolo; V. Paeder; V. Musi; F. Giorgis, and E. Descrovi, Bloch surface waves-controlled emission of organic dyes grafted on a one-dimensional photonic crystal. *Applied Physics Letters* 99, 043302 (2011). doi:10.1063/1.3616144
- [2] A. Angelini; E. Barakat; P. Munzert; L. Boarino; N. De Leo; E. Enrico; F. Giorgis; H.P. Herzig; C.F. Pirri; E. Descrovi, Focusing and Extraction of Light mediated by Bloch Surface Waves. *Scientific Reports*. 4, 5428 (2014). doi:10.1038/srep05428
- [3] R. Badugu; K. Nowaczyk; E. Descrovi; J.R. Lakowicz, Radiative decay engineering 6: Fluorescence on one-dimensional photonic crystals. *Analytical Biochemistry* 442, 83 (2013). doi:10.1016/j.ab.2013.07.021
- [4] U.Stella; L. Boarino; N. De Leo; P. Munzert; E. Descrovi, Enhanced directional light emission assisted by resonant Bloch Surface Waves in circular cavities, manuscript in preparation

**Session B6**

**15:00 - 15:30 PM Room B December 18**

**B18: High-dimensional vectorial holographic encryption with metasurfaces**

Lingling Huang\*

*School of Optics and Photonics, Beijing Institute of Technology, Beijing, 100081, China*

\*Corresponding author. Email: huanglingling@bit.edu.cn

**Abstract**

Holography based on metasurfaces has emerged as a promising candidate for applications in optical displays, optical storage and security by exhibiting unprecedented spatial resolution, enormous information capacity and large field of view compared to traditional methods. For exploring the full capability of the information storage/display and enhance the encryption security of metasurface holograms, smart multiplexing techniques together with suitable metasurface designs are highly demanded. Here we integrate multiple polarization manipulation channels for various spatial phase profiles into a single birefringent vectorial hologram by completely avoiding unwanted cross-talk. Multiple independent target phase profiles with quantified phase relations that can process significantly different information in different polarization states are realized within a single metasurface. For our metasurface holograms, we demonstrate high fidelity, large efficiency, broadband operation, and a total of twelve polarization channels. Such multichannel polarization multiplexing can be used for dynamic vectorial holographic display and provide triple protection to the optical security. The concept is appealing for applications of arbitrary spin to angular momentum conversion and various phase modulation/beam shaping elements.

**Keywords**

Holography; metasurfaces

**References**

[1] Zhao, R., Sain, B., Wei, Q., Tang, C., Li, X., Weiss, T., Huang, L.\*, Wang, Y.\*, Zentgraf, T.\* Multichannel Vectorial Holographic Display and Encryption. *Light: Science & Applications* (2018)

**Session B7**

**16:00 - 16:30 PM Room B December 18**

## **B19: Applications of transferable ZTO nanospheres monolayer to optoelectronic devices**

Jinsub Park<sup>1,2,\*</sup>, Uijin Jung<sup>1</sup>, Dong Su Shin<sup>1</sup>, Dohyun Kim<sup>1</sup>

<sup>1</sup>Department of Electronics and Computer Engineering, Hanyang University, Seoul 04763, Republic of Korea

<sup>2</sup>Department of Electronics and Computer Engineering, Hanyang University, Seoul 04763, Republic of Korea

\*Corresponding author. Email: jinsubpark@hanyang.ac.kr

### **Abstract**

Zinc-tin-oxide (ZTO) has been considered as attractive optoelectronic materials due to their physical and chemical properties. [1] Recently many groups reported that the various phases of ZTO effect on their device performances in versatile applications such as anodes of battery, [2] active layer in transistor, photovoltaic devices, photodetector [3], and gas sensors based on the outstanding properties. Here, we report on the formation of transferable nano/microspheres monolayers consisting of ZnSnO<sub>3</sub> (ZTO) synthesized by fast ethanol precipitation and their application to GaN-based light-emitting diodes (LEDs) to improve the electrical and optical device performances. ZTO microspheres with different diameters of 800, 900, 1200 nm were synthesized and arrayed to form a monolayer using polydimethylsiloxane (PDMS) and simple rubbing method. The formed monolayers show the optical transmittance percentages of 94, 93, and 87 % at 460 nm, respectively. Effects of ZTO monolayers on the light extraction efficiency of LEDs were evaluated using fabricated LED chips. All LEDs with ZTO monolayer as a top-layer show improvement of light extraction efficiency about 120 ~ 145% relative to regular LEDs as well as enhanced electrical properties as evidenced by a decrease in turn on voltage. The XPS analysis indicated that the improvement in the electrical properties of LEDs with ZTO monolayers is related to the presence of graphene-like carbon bonds present in carbon residue that remains on the surface of the LED after removal of polymer. The improvement of light extraction using ZTO nano/microspheres monolayer on LEDs can be attributed to effective guiding of light generation from active regions in LEDs towards air, which was confirmed by theoretical simulations.

### **Keywords**

ZTO nano/micro spheres; LED; Extraction efficiency; Monolayers

### **References**

- [1] Sun, S., & Liang, S. Morphological zinc stannate: synthesis, fundamental properties and applications. *J. Mater. Chem.* 5(39), 20534(2017)
- [2] Hou, X., Cheng, Q., Bai, Y., & Zhang, W. F. Preparation and electrochemical characterization of Zn<sub>2</sub>SnO<sub>4</sub> as anode materials for lithium ion batteries. *Solid State Ionics*, 181, 631 (2010)
- [3] Bera, A., Sheikh, A. D., Haque, M. A., Bose, R., Alarousu, E., Mohammed, O. F., & Wu, T. Fast crystallization and improved stability of perovskite solar cells with Zn<sub>2</sub>SnO<sub>4</sub> electron transporting layer: interface matters. *ACS appl. Mater. Inter.* 7, 28404(2015)

**Session B7**

**16:30 - 17:00 PM Room B December 18**

**B20: Development and characterization of metallo-dielectric nanomaterials**

Yan Hong<sup>1,\*</sup>, Bjoern M Reinhard<sup>2</sup>

<sup>1</sup>University of Electronic Science and Technology of China, Chengdu, Sichuan, 610054, China

<sup>2</sup>Department of Chemistry & Photonics Center, Boston University, Boston, Massachusetts 02215, United States

\*Corresponding author. Email: hongyan@uestc.edu.cn

**Abstract**

This talk covers the work of rational combination from dielectric and metallic nano components. The concept of ‘optoplasmonic’ materials referring to the entities embracing the interaction between plasmonic fields and peripheral photonic landscape will be particularly stated in the presentation [1]. As for fabrication, template-assisted self-assembly approaches are conducted to build up nano complex with titanium dioxide and gold nano spheres. A top-bottom hybrid unit and interdigitated hybrid array are achieved [2-3]. With the characterization of the elastic and inelastic spectra of these heterogeneous materials, physical models are computed to depict the scenario of varied geometry and combination of nano particles. In sharp contrast to purely dielectric or metallic particle arrays, this artificial-material not only enhances the electric near field intensity in the cavity of metal nano cluster ‘hot spots’, but also expands the volume of enhanced electric field. Further research reveals that the extra enhancement and redistribution of near field are originated from the coupling between the localized plasmon resonance and the in-plane photonic mode of the companion dielectric array [4].

**Keywords**

2D nanomaterial; Plasmonic material; gold nanoparticle; SERS; photonic array

**References**

- [1] Y. Hong, W. Ahn, S. V. Boriskina, X. Zhao, B.M. Reinhard, Directed Assembly of Optoplasmonic Hybrid Materials with Tunable Photonic-Plasmonic Properties, *J. Phys. Chem. Lett.*, 6, 2506 (2015). doi: 10.1021/acs.jpcclett.5b00366
- [2] Y. Hong, M. Pourmand, S. V. Boriskina, B.M. Reinhard, “Enhanced Light Focusing in Self-Assembled Optoplasmonic Clusters with Subwavelength Dimensions”, *Adv. Mater.*, 25, 115 (2013). doi: 10.1002/adma.201202830
- [3] Y. Hong, Y. Qiu, T. Chen, B. M. Reinhard, “Rational Assembly of Optoplasmonic Hetero-nanoparticle Arrays with Tunable Photonic–Plasmonic Resonances”, *Adv. Funct. Mater.*, 24, 721 (2014). doi: 10.1002/adfm.201301837
- [4] Y. Hong, B.M. Reinhard, “Collective Photonic-Plasmonic Resonances in Noble Metal – Dielectric Nanoparticle Hybrid Arrays”, *Opt. Mater. Express*, 4, 2409 (2014). doi:10.1364/OME.4.002409



**Session B7**

**17:00 - 17:30 PM Room B December 18**

**B21: Electrons dynamics control in ultrafast laser micro/nanofabrication by spatially/temporally shaped pulses**

Xiaowei Li<sup>1</sup>, Lan Jiang<sup>1,\*</sup>, Yongfeng Lu<sup>2</sup>

<sup>1</sup>*Laser Micro/Nano Fabrication Laboratory, School of Mechanical Engineering, Beijing Institute of Technology, Beijing, 100081, China*

<sup>2</sup>*Department of Electrical and Computer Engineering, University of Nebraska-Lincoln, Lincoln, NE 68588-0511, USA*

Email: jianglan@bit.edu.cn

**Abstract**

An ultrafast laser pulse duration is shorter than many physical/chemical characteristic times, which makes it possible to manipulate/adjust electron dynamics, such as excitation and ionization of electrons. By spatially/temporally shaping femtosecond laser pulses, localized transient electron dynamics are actively controlled during laser-material interactions. A multiscale model is developed, which consists of the ab initio calculations for electrons dynamics, revised molecular dynamics simulation for phase change, plasma model for ionization processes, and improved two-temperature model for energy transport. Our simulation shows that it is feasible to control electron dynamics to adjust localized transient material properties, phase changes, and micro/nanostructures. Using the proposed mechanism, high-quality microholes with a diameter of 1.5  $\mu\text{m}$  and an aspect ratio of 1000:1 are fabricated by a shaped single femtosecond laser pulse. It takes 42 min to fabricate 251,001 holes in a 1 cm  $\times$  1 cm area, which is very uniform in size and shape. A multiscale measurement system (from femtosecond scale to second scale) is developed for high-quality, high-aspect-ratio drilling using a femtosecond laser. It consists of a pump-probe shadowgraph imaging technique, laser-induced breakdown spectroscopy (LIBS), and an intensified charge-coupled device (ICCD) camera. For the first time, we reveal the multiple time scale fundamentals during femtosecond laser material interactions, including the femtosecond-scale propagation of a laser pulse, picosecond-scale generation/evolution of laser-induced plasma, nanosecond-scale plasma ejection/expansion, and microsecond-scale hole formation.

**Keywords**

Ultrafast laser micro/nanofabrication; electron dynamics; multiscale measurement

**References**

- [1] L. Jiang, A. Wang, B. Li, T. Cui, Y. Lu, *Light: Sci. & Appl.*, 7 (2), 174134 (2018)
- [2] L. Jiang, P. Liu, X. Yan, N. Leng, C. Xu, H. Xiao, Y. Lu, *Opt. Lett.* 37, 2781-2783 (2012)
- [3] Z. Yao, L. Jiang, X. Li, A. Wang, Z. Wang, M. Li, Y.F. Lu, *Opt. Express*, 26, 21960-21968 (2018)
- [4] A. Wang, L. Jiang, X. Li, Y. Liu, X. Dong, L. Qu, X. Duan, Y. Lu, *Adv. Mater.* 27, 6238-6243 (2015)

**Session B7**

**17:30 - 18:00 PM Room B December 18**

## B22: Plasmon-enhanced nanoscopy for nanoscale analysis

Taka-aki Yano<sup>1,2,\*</sup>

<sup>1</sup>*School of Materials and Chemical Technology, Tokyo Institute of Technology, Yokohama 226-8502, Japan*

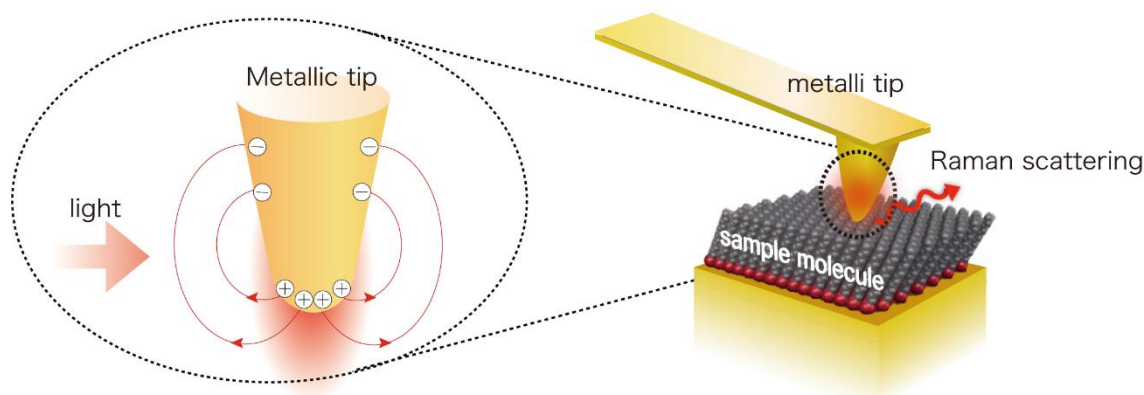
<sup>2</sup>*RIKEN, Wako, Saitama 351-0198, Japan*

\*Corresponding author. Email: yano@echem.titech.ac.jp

### Abstract

Tip-enhanced Raman scattering (TERS) microscopy, a family of scanning probe microscopy techniques, has been recognized as a powerful surface analytical technique with both single-molecule sensitivity and nanoscale spatial resolution far beyond the diffraction limit of light. Recently, we have proposed to utilize a metallic probe tip not only to locally excite Raman scattering from sample molecules, but also to locally apply external stimuli to the molecules through the tip apex. The tip-applied stimuli including pressure, voltage, and temperature are likely to induce structural and conformational changes, band-gap tuning, and photochemical reactions in the vicinity of the tip apex. Combination of TERS microscopy with the local external stimuli has now opened up a new way to control molecular properties and functions on a nanometer scale along with the in situ nano-analysis, which can contribute to active functional control of nanodevices.

If time allows, we will extend the topic to non-plasmonic nanophotonics with the use of high-index dielectric nanostructures which have been recently regarded as an alternative to plasmonic nanostructures.



### Keywords

Plasmonics; Nanophotonics; Dielectric nanostructures; Field-enhanced spectroscopy

**Session A8**

**9:00 - 9:30 AM Room A December 19**

**A22: Multiscale modeling of heat transfer in low-dimensional materials**

Yuan Dong<sup>1,\*</sup>, Zengyuan Guo<sup>2</sup>

<sup>1</sup>*Department of Mechanical & Aerospace Engineering, University of Missouri, Columbia, Missouri 65211 United States*

<sup>2</sup>*Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China*

\*Corresponding author. Email: dongyu@missouri.edu

**Abstract**

The heat transfer in low-dimensional materials is very important and intriguing phenomena containing the following non-trivial effects: The strong boundary scattering induced thermal conductivity reduction and the low-dimensional effect induced thermal conductivity enhancement. Understanding the underlying mechanism and building reliable models for such heat transfer are critical for the applications in advanced chip cooling, high efficient thermal electrics as well as other energy related nanomaterials. Here we present our work in recent years which targeted on the multiscale modelling of nanoscale heat transfer. The first principles calculation is on the electron scale. The molecular dynamics simulation is on the atomic and molecular scale. The phonon gas model based on the thermomass theory is on the mesoscopic scale. Bridge these scales we have developed a series of fundamental understanding and engineering applicable models, which enhance our capability to harness the energy flow in nanoscale.

**Keywords**

Multiscale Modeling; Low-Dimensional Materials; Thermomass theory; DFT; Molecular dynamics

**Session A8**

**9:30 - 10:00 AM Room A December 19**

**A23: Advanced materials and processes for Silicon based solar cells**

Rosaria Puglisi\*

*Institute for Microelectronics and Microsystems, Italy*

\*Corresponding author. Email: [rosaria.puglisi@imm.cnr.it](mailto:rosaria.puglisi@imm.cnr.it)

**Abstract**

The activity concerns the synthesis, fabrication and characterization of materials and solar cells based on innovative structures and advanced processes. New three dimensional architectures are chosen because they allow to improve the photoconversion efficiency of Si by increasing the light absorption or by decoupling the photons path from the photogenerated carriers collection. Si nanowires deposited in a plasma-based Chemical Vapor Deposition (CVD) system, by vapor-liquid-solid method catalysed through metallic nanodots, are integrated in the emitter of the cell as light trapping layer.

In addition to the most popular 3D architectures, such as the wires, the potential of other innovative geometries like Si Nanoholes (NH) are exploited. These have recently been proved as a promising alternative to the positive counterparts, thanks to their better mechanical robustness during process integration and to their good optical match with visible light. As a main enabling technology for the synthesis of the Si NHs the nanolithography based on self-assembling of diblock copolymers is used. Another important technology developed in the last years and exploited in the present activity is the monolayer doping for the formation of ultra-thin and conformal silicon junctions. The research topics relate to various aspects of the formation of a solar cell: from the 3D structures synthesis to the junction formation process, to the structural and electro-optical characterization, and the devices are fabricated in-house starting from the Si substrate up to the complete device. The activity is complemented by the simulation of the advanced processes applied for the synthesis of the nanostructures. In particular, the simulation of the plasma condition in the equipment used for the growth processes aids the understanding and control of the synthesis of the positive 3D structures. Dopant atoms transfer from the molecular systems mechanism is also modeled and impurity profiles are simulated by varying the process conditions.

Another important focus is on the study of the materials synthesized by plasma based CVD. The plasma technology is particularly appreciated for its compatibility with device production lines and its flexibility in terms of throughput. We exploit the capabilities of plasma to produce advanced materials, such as Si based and C based materials, optionally doped with P or B, like amorphous Si, SiC and oxynitrides/oxycarbide SiO<sub>x</sub>N<sub>y</sub>C<sub>z</sub>, for several applications in photovoltaics.

**References**

[1] <https://hq.imm.cnr.it/articles/silicon-solar-cells-based-advanced-architectures-and-processes>

**Session A8**

**10:00 - 10:30 AM Room A December 19**

**A24: Vacancy diffusion in graphene**

Mukul Kabir\*

*Department of Physics, Indian Institute of Science Education and Research, Pune, India*

\*Corresponding author. Email: mukul.kabir@iiserpune.ac.in

**Abstract**

The interaction between the spatially scattered vacancy defects and their kinetics drive various structural modifications, which severely alter the electronic, magnetic and transport properties. Thus, understanding the microscopic vacancy diffusion in a device setup becomes important. In this regard, we will discuss the dynamic Jahn-Teller distortion and vacancy diffusion with different carrier doping. [1] We will demonstrate that lattice relaxation perpendicular to the graphene sheet and in-plane strain relaxation play the predominant roles in predicting the correct microscopic mechanism for vacancy diffusion and thus the accurate activation barrier. We will show that the calculated activation barrier increases upon both electron and hole doping and the observed trends are explained by the differential charge density and by the hardening of the low-energy phonon modes that are responsible for vacancy diffusion. Electron doping essentially freezes the vacancy, and thus any degradation mediated by it through a dramatic decrease in diffusivity. While tracking vacancy diffusion experimentally in graphene is a difficult task, the present results will motivate new experimental efforts and assist interpretation of the results. In this talk, we will also discuss the importance of the quantum correction to the classical barrier.

**References**

[1] Rohit Babar and Mukul Kabir, *Gate-dependent vacancy diffusion in graphene*, Physical Review B 98, 075439 (2018)

**Session A9**

**11:00 - 11:30 AM Room A December 19**

**A25: Chirality Effects on an Electron Transport in Single-walled Carbon Nanotube**

S. Boonchui<sup>1,\*</sup>, J. Charoenpakdee

*Department of Physics, Kasetsart University, Bangkok, 10900, Thailand*

\*Corresponding author. Email: fscistb@ku.ac.th

**Abstract**

We investigate that conductivity depend on the direction of current due to the chirality of each chiral's index single-wall carbon nanotubes (SWCNTs). According to the asymmetric velocities of Dirac particles calculated by inducing curvature-induced  $\sigma$ - $\pi$  mixing and Slater-Koster type projection for  $\pi$ - $\pi$  and  $\sigma$ - $\pi$  hopping integrals, we provide an analytical expression by calculating the current-current correlation function for the paramagnetic and diamagnetic current density operator. The current-current correlation function as a function of the energy for different directions of bias voltage are discussed for the chiral index.

**Keywords**

Carbon nanotube; chirality; the current-current correlation; the paramagnetic and diamagnetic current

**References**

- [1] F. Qin, W. Shi, T. Ideue, M. Yoshida, A. Zak, R. Tenne, T. Kikitsu, D. Inoue, D. Hashizume and Y. Iwasa, Superconductivity in a chiral nanotube. *Nature Commun.* 8, 14465 (2017)
- [2] Vasilii I. Artyukhov, Evgeni S. Penev and Boris I. Yakobson, Why nanotubes grow chiral. *Nature Commun.* 5, 4892 (2014)
- [3] Van Hieu Nguyen, Bich Ha Nguyen and Ngoc Dung Dinh, Theory of Green function of free Dirac fermions in graphene. *Adv. Nat. Sci.: Nanosci Nanotechnol.* 7, 015013 (2016)
- [4] J. Sabio, J Nilsson, and A. H. Castro Neto, f-sum rule and unconventional weight transfer in graphence. *Phys. Rev. B* 78, 075410 (2008)

**Session A9**

**11:30 - 12:00 PM Room A December 19**

**A26: Ionic liquids assisted synthesis of porous carbon materials for energy storage devices**

Yang Yan\*, Xiao-Feng Hao, Nan Cui, Zhen-zhen Pan, Ce Hao

*School of Petroleum and Chemical Engineering, Dalian University of Technology • Panjin, Panjin, Liaoning 124221, China*

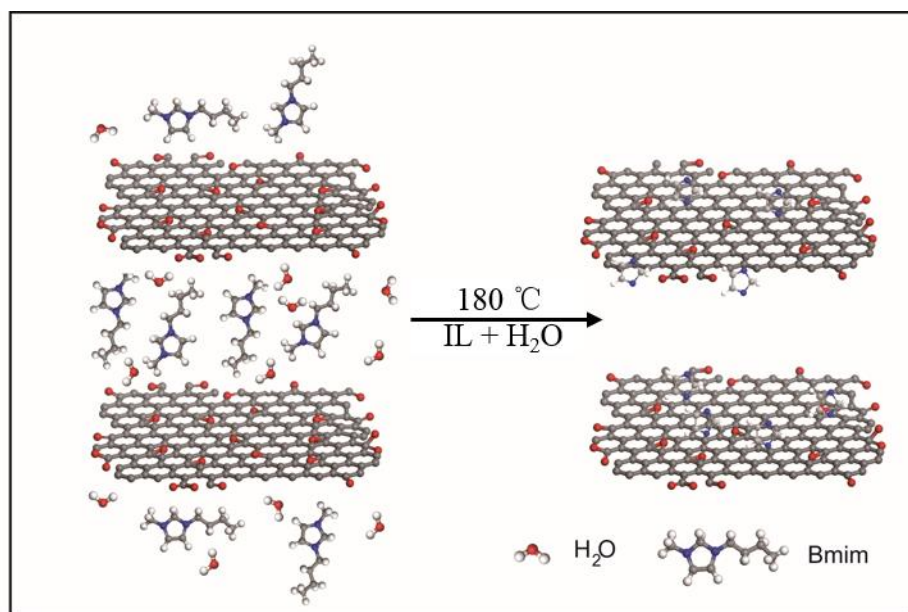
\*Corresponding author. Email: yanyang@dlut.edu.cn

**Abstract**

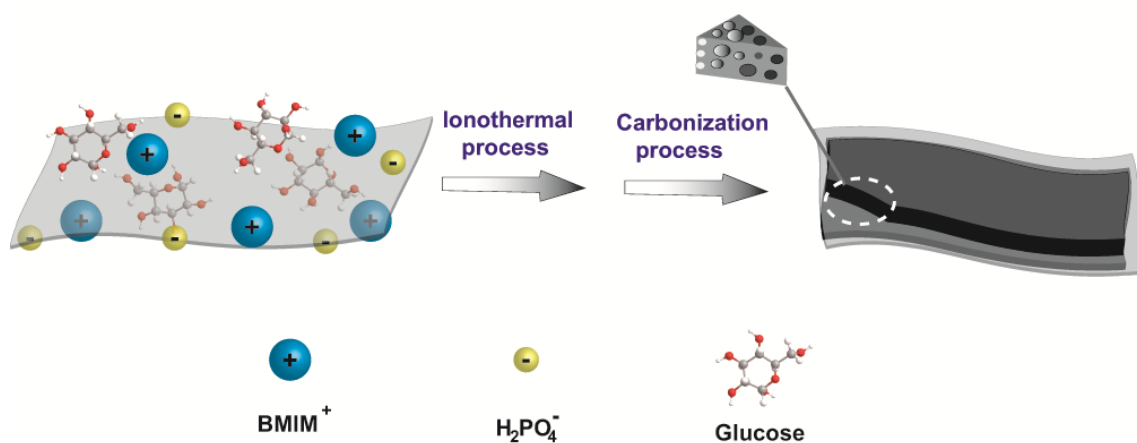
Electrochemical energy storage with high energy density and high power density is highly demanded for portable electric devices, electric vehicles and smart grids. Rechargeable batteries and supercapacitors have been extensively studied and used in the field of electric devices. Porous carbon materials play great roles in those energy storage systems for its low cost, chemical stability and high conductivity. However, the commonly used method for synthesizing carbon materials suffers from some drawbacks, such as multistep, time consuming and pollution problems. Moreover, the widely investigated graphene-based carbon materials aggregate seriously due to the  $\pi$ - $\pi$  stacking.

Ionic liquids (ILs), composed of cations and anions, are attracting considerable attentions due to their unique properties, such as strong dissolution, non-volatility, high thermal stability, low flash point and high polarity. Such a wide range of unique properties endow ILs as suitable alternatives for the synthesis of engineered materials by acting as advanced solvents, dopants, and templating agents.

Thus, we proposed an ionic liquid-assisted method to prepare graphene-based carbon materials for supercapacitors and rechargeable batteries. Firstly, fabricated a 3D reduced graphene oxide (ILG) by one-step ionic liquid induced self-assembly method (Scheme 1) and constructed a flexible symmetric supercapacitor with the obtained ILG. The IL plays great roles of a protector and stabilizer. The obtained ILG shows high specific capacitance ( $260 \text{ F g}^{-1}$  at  $0.5 \text{ A g}^{-1}$ ), superior rate capability in both 6 M KOH electrolyte and symmetric all-solid-state supercapacitor. Secondly, we synthesized a graphene-based hierarchically porous carbon (GPC) by ionothermal method and constructed supercapacitor with IL electrolyte as shown in Scheme 2. The GPC electrode exhibits a high energy density of  $90.4 \text{ Wh kg}^{-1}$ , highlighting the application of IL electrolyte in EDLCs. Except for the supercapacitors, we also designed graphene-based nanocomposite ( $\text{Sb}_2\text{S}_3/\text{rGO}$ ) by ionic liquid-assisted method for sodium ion batteries. The ionic liquid plays a great role in stabilizing the graphene oxide and facilitating the formation of uniform coating of  $\text{Sb}_2\text{S}_3$  on rGO. The as-prepared IL- $\text{Sb}_2\text{S}_3/\text{rGO}$  exhibits an impressive specific capacity of  $687.7 \text{ mA h g}^{-1}$  at a current density of  $50 \text{ mA g}^{-1}$  and a high-rate capability as an anode for sodium ion batteries.



**Scheme 1.** Schematic diagrams of the ILG synthesis route



**Scheme 2.** Fabrication schematic of graphene-based hierarchically porous carbon (GPC)

**Keywords**

Ionic liquid; carbon material; graphene-based; supercapacitor; batteries

**References**

- [1] D. C. Guo, J. Mi, and A. H. Lu, Energy Environ. Sci.,2013,6,652-659
- [2] S.G. Zhang, K.Dokko and M. Watanabe, Mater. Horiz., 2015,2,168-197
- [3] Y. Yan, N. Cui and C. Hao, J. Alloy. Compu.,2019,776,22-30
- [4] X. F. Hao, Y. Yan and C Hao. Electrochimica Acta, 2017, 241,124-131
- [5] Z. Pan, Y. Yan and C. Hao, Adv. Mater. Interfaces, 2018, 1701481



**Session A9**

**12:00 - 12:30 PM Room A December 19**

## **A27: Dual-Functional Templated Methodology for the Synthesis of Hierarchical Porous Carbon for Supercapacitor**

Feng Shen\*, Xinhua Qi

*Agro-Environmental Protection Institute, Chinese Academy of Agricultural Sciences, No. 31, Fukang Road, Nankai District, Tianjin, China*

\*Corresponding author. Email: shenwindy@126.com

### **Abstract**

Dual-functional templated methodology was developed for synthesis of hierarchical porous carbons via direct thermal decomposition of agricultural wastes, in which dairy manure acted as low cost carbon precursor and eggshell as both hard template and activating agent source of CO<sub>2</sub>. The dual-functional template can be easily removed by diluted HCl instead of corrosive HF. Carbonization temperature and dosage of eggshell have great influence on the porous texture of the carbon materials. Optimized temperature of 800 °C and mass ratio of eggshell/dairy manure (2:1) facilitate the releasing of CO<sub>2</sub> from eggshell thus benefitting the formation of hierarchical porous carbon. The porous carbon has maximum surface area of 543.6 m<sup>2</sup>/g and total pore volume of 0.48 cm<sup>3</sup>/g of which micropores account for 40%. As the electrode of supercapacitor, the obtained hierarchical porous carbons showed a relative high specific capacitance of 226.6 F/g in KOH aqueous electrolyte (6 mol/L). Besides, it exhibited outstanding cycling stability with almost 100% of specific capacitance retention after 2500 GCD cycles. The one-step template carbonization method provides a facile and sustainable route to prepare hierarchical porous carbons from the agricultural wastes.

### **Keywords**

Dual-functional template; Eggshell; Dairy manure; Porous carbon; Supercapacitor

### **References**

- [1] K. T. Cho; B. L. Sang; J. W. Lee, Facile synthesis of highly electrocapacitive nitrogen-doped graphitic porous carbons. *Journal of Physical Chemistry C* 118, (2014), 9357. doi:10.1021/jp501742x
- [2] J. Lee; J. Kim; T. Hyeon, Recent progress in the synthesis of porous carbon materials. *Advanced Materials* 18, (2006) 2073. doi:10.1002/adma.200501576
- [3] L. Zhu; F. Shen; R. L. Smith; X. Qi, High-performance supercapacitor electrode materials from chitosan via hydrothermal carbonization and potassium hydroxide activation. *Energy Technology* 5, (2016), 452. doi: 10.1002/ente.201600337

**Session A10**

**14:00 - 14:30 PM Room A December 19**

**A28: Intrinsic field effect and Hall mobility in multilayer III-VI 2D semiconductor InSe FETs**

Sukrit Sucharitakul<sup>1</sup>, Nicholas J. Goble<sup>1</sup>, U. Rajesh Kumar<sup>1,4</sup>, Raman Sankar<sup>3</sup>, Zachary Bogorad<sup>5</sup>, Fang Cheng Chou<sup>3</sup>, Yit-Tsong Chen<sup>2,4</sup>, Xuan P. A. Gao<sup>1,\*</sup>

<sup>1</sup>*Department of Physics, Case Western Reserve University, 2076 Adelbert Road, Cleveland OH 44106*

<sup>2</sup>*Department of Chemistry and* <sup>3</sup>*Center for Condensed Matter Sciences, National Taiwan University, Taipei*

<sup>4</sup>*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei*

<sup>5</sup>*Solon High School, 33600 Inwood Dr, Solon, OH 44139*

\*Corresponding author. Email: sukrit.sucharitakul@riken.jp

**Abstract**

Graphene-like two-dimensional (2D) materials, not only are interesting for their exotic electronic structure and fundamental electronic transport or optical properties but also, hold promises for device miniaturization down to atomic thickness. As one material belonging to this category, InSe is not only a promising candidate for optoelectronic devices but also has potential for ultrathin field effect transistor (FET) with high mobility transport. In this work, various substrates such as PMMA, bare silicon oxide, passivated silicon oxide, and silicon nitride were used to fabricate multi-layer InSe FET devices. Through back gating and Hall measurement, the devices' field effect mobility and intrinsic Hall mobility were extracted at various temperatures to study the material's intrinsic transport behavior and the effect of dielectric substrate. Overall trend of the devices' mobility was found to increase as the temperature is reduced due to reduced phonon scattering. The sample's field effect and Hall mobilities over the range of 77-300K fall in the range of  $0.1-2.0 \times 10^3 \text{ cm}^2/\text{Vs}$ , better than FETs made of more widely studied 2D transition metal-dichalcogenides.

**Keywords**

2D material; InSe; FET; mobility; thin film

**Session A10**

**14:30 - 15:00 PM Room A December 19**

**A29: Nano-enabled clean water production by sunlight**

Peng Wang\*

*King Abdullah University of Science and Technology, Saudi Arabia*

\*Corresponding author. Email: peng.wang@kaust.edu.sa

**Abstract**

Given the vast abundance and inexhaustibility of sunlight, tapping into solar energy to produce clean water seems a viable solution to current global challenges of water scarcity and clean energy shortage. Solar driven water evaporation, which uses photothermal materials to capture and convert sunlight to heat so to generate water vapor, is an ancient process and integral part of any solar powered clean water production. The old concept of utilizing solar-driven water evaporation to produce clean water resurfaced and was rejuvenated over the past five years because it uses only sunlight without any CO<sub>2</sub> emissions during the operation. The rejuvenation of the photothermal processes in the new times gains very helpful hand from nanomaterials. In this presentation, various nano-enabled photothermal materials that are able to capture whole solar spectrum and convert it to heat with almost 100% efficiency will be covered. The recent development in rationally designed photothermal structures with proper heat loss management that has led to the solar-driven water evaporation efficiency being steadily and significantly improved in the last three years, from ~50% to a near 100%, will be presented.

**Session A10**

**15:00 - 15:30 PM Room A December 19**

## A30: Thin Graphite Contact for 2D-Layered Material CMOS Device and Band Gap Estimation

June Yeong Lim<sup>1</sup>, Sam Park<sup>1</sup>, Sanghyuck Yu<sup>1</sup>, Jungcheol Kim<sup>2</sup>, Hyeonsik Cheong<sup>2</sup>, Seongil Im<sup>1,\*</sup>

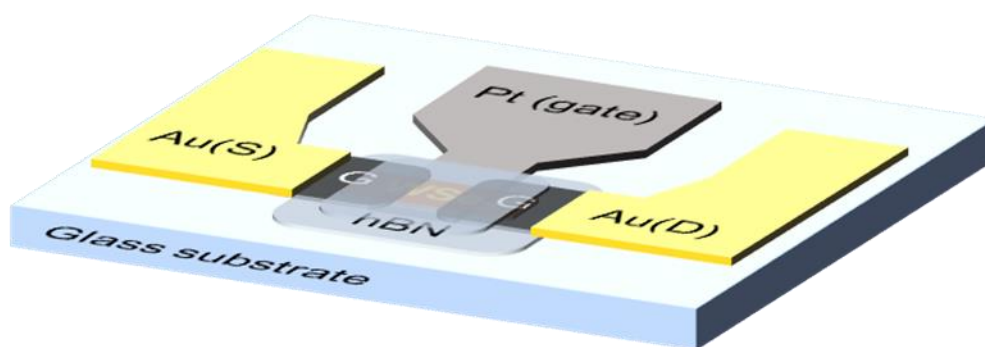
<sup>1</sup>Department of Physics, Yonsei University, Seoul, Republic of Korea

<sup>2</sup>Department of Physics, Sogang University, Seoul, Republic of Korea

\*Corresponding author. Email: semicon@yonsei.ac.kr

### Abstract

Band gap of monolayer and few layers in two dimensional (2D) semiconductors has usually been measured by optical probing such as photoluminescence (PL). However, if their exfoliated thickness is as large as a few nm (multilayer over  $\sim 5L$ ), PL measurements become less effective and inaccurate because the optical transition of 2D semiconductor is changed from direct to indirect mode. Here, we introduce another way to estimate the bandgap of multilayer 2D van der Waals semiconductors; that is utilizing field effect transistor (FET) as a platform. We used graphene (thin graphite) contact for multilayer van der Waals channels in FET, because graphene contact would secure ambipolar behavior and enable Schottky contact barrier tuning of FETs with the assistance of top passivation. As a result, the bandgaps of multilayer transition metal dichalcogenides and black phosphorus in unknown thickness were successfully estimated through measuring the temperature-dependent transfer curve characteristics of prepared 2D FETs with graphene contact. Furthermore, based on these thin graphite contact, we also have successfully fabricated all 2D layered material-based CMOS inverter with n-MoS<sub>2</sub> and p-MoTe<sub>2</sub> channels, and demonstrate its device properties.



### References

- [1] K. Choi, Y. T. Lee, J. S. Kim, S. W. Min, Y. Cho, A. Pezeshki, D. K. Hwang and S. Im, *Adv. Funct. Mater.*, 2016, 26, 3146–3153
- [2] Y. T. Lee, K. Choi, H. S. Lee, S. W. Min, P. J. Jeon, D. K. Hwang, H. J. Choi and S. Im, *Small*, 2014, 10, 2356–2361

***Session A11***

***16:00 - 16:30 PM Room A December 19***

**A31: Energy dissipation and light emission in graphene**

Myung-Ho Bae\*

*Korea Research Institute of Standards and Science, Republic of Korea*

\*Corresponding author. Email: mhbae@kriss.re.kr

**Abstract**

Energy dissipation in nanoscale electronics has become an important subject in modern electronic industry and energy conversion system. From this perspective, graphene with very high mobility and thermal conductivity, which are about ten times higher than silicon, is a very attractive nano-material to study energy dissipation in nano-electronics. I will present studies for the tunable Heat transport and light emission in graphene devices.

**Session A11**

**16:30 - 17:00 PM Room A December 19**

**A32: Unexpectedly Promoting Effect of Carbon Nanotubes Grown During the Non-oxidative Coupling of Methane over Copper Catalysts**

Zhi-Yen Zeng<sup>1</sup>, Jian Chen<sup>2</sup>, Jarrn-Horng Lin<sup>1,\*</sup>

<sup>1</sup>Department of Materials Science, National University of Tainan, 33, Sec. 2, Shu-lin St., Tainan

<sup>2</sup>Department of Materials Science and Engineering, Sichuan University of Science and Engineering, Key Lab Material Correction and Protection, Zigong, 643000, China

\*Corresponding author. Email: janusjhlin@mail.nutn.edu.tw

**Abstract**

One of the challenges for the non-oxidative coupling of methane (NOCM) is to effectively remove the deposited coke over catalysts owing to the over-dehydrogenation of methane. Herein, we show that an in-situ growth of carbon nanotubes (CNTs) instead of coke were observed during NOCM over a  $\text{CuSO}_{4/\gamma}\text{-Al}_2\text{O}_3$  catalyst. The as-grown CNTs depict an unexpected promoting effect for NOCM with a highest activity of  $0.48 \text{ mol kg cat}^{-1}\cdot\text{h}^{-1}$ , and maintained 85% activity after 200 h running time. The equilibrium methane conversion is 9.8 % with a selectivity of 78.2 % for  $\text{C}_2$  ( $\text{C}_2\text{H}_4 + \text{C}_2\text{H}_6$ ) products. Highly dispersed Cu nanoparticles distributed on the top of CNTs measured by transmission electron microscopy is proposed to result in high catalyst stability during NOCM for 200h instead of deactivation in several hours. Here, we firstly prove that the as-grown CNTs can promote the catalytic activity of NOCM instead of deactivation by coking over catalysts.

**Keywords**

Carbon nanotube; Non-oxidative coupling of methane; Copper catalysts; Promoting effect; Catalytic activity

**Session B8**

**9:00 - 9:30 AM Room B December 19**

## **B23: Micro and nanocoatings for biomedical applications improving Ti50Zr alloy performance**

Ioana Demetrescu<sup>1,2,\*</sup>

<sup>1</sup>General Chemistry Department, University POLITEHNICA of Bucharest, 1-7 Polizu Str., Bucharest, Romania

<sup>2</sup>Academy of Romanian Scientists, 54 Splaiul Independentei, Bucharest, Romania

\*Corresponding author. Email: i\_demetrescu@chim.upb.ro

### **Abstract**

The presentation contains new results regarding the properties of micro and nanocoatings fabricated on Ti50Zr in the context of the new trend to extend Zr alloys use for restorative works especially in the oral cavity. According to investigations of TiZr with various Zr content, Ti50Zr was a better choice to reach performance taking into account that TiZr stability is increasing with Zr content only until 50%. For higher Zr content, its stability in bioliquids is decreasing [1]. The Ti50Zr was coated via various procedures obtaining micro and nano architectures as a function of fabrication method. Microstructures were fabricated via electrochemical deposition of a mixture of chitosan and hydroxyapatite [2]. Nanocoatings were fabricated via one [3] or two steps anodizing [4] protocols and by changing anodizing conditions and posttreatments. The structure, morphology, topography, hydrophilic character, and biological aspects were evaluated and discussed. The AFM investigations developing more knowledge about adhesive and nanomechanical properties were used as a tool in understanding the interface. The mainly evidenced biological aspects were cell viability, NO and ROS levels. The biological assays were completed with the investigation of the antibacterial ability of the coatings. The results were correlated with the coatings properties and discussed as an expression of bioperformance.

### **Keywords**

Performance of bionic coating of chitosan and hydroxyapatite; Surface properties of Ti50Zr nanotubes; AFM nanomechanical properties; Biological assays: cell viability, NO, ROS, antibacterial effect

### **References**

- [1] T. Akimoto, T. Ueno, Y. Tsutsumi, H. Doi, T. Hanawa, N. Wakabayashi, Evaluation of corrosion resistance of implant-use Ti-Zr binary alloys with a range of compositions. *Journal of Biomedical Materials Research Part B: Applied Biomaterials*. 106, 73 (2018). doi: 10.1002/jbm.b.33811
- [2] M. Vardaki, D. Ionita, A. B. Stoian, I. Demetrescu, Increasing corrosion resistance of a ZrTi alloy with a bioinspired coating with low porosity. *Materials and Corrosion*. 68, 988 (2017). doi: 10.1002/maco.201609408
- [3] A. B. Stoian, M. Vardaki, D. Ionita, M. Enachescu, M. Prodana, O. Brancoveanu, I. Demetrescu, Nanopores and nanotubes ceramic oxides elaborated on titanium alloy with zirconium by changing anodization potentials. *Ceramics International*. 44, 7026 (2018). doi: 10.1016/j.ceramint.2018.01.137
- [4] S. Grigorescu, C. Ungureanu, R. Kirchgeorg, P. Schmuki, I. Demetrescu, Various sized nanotubes on TiZr for antibacterial surfaces. *Applied Surface Science*. 270, 190 (2013). doi: 10.1016/j.apsusc.2012.12.165

**Session B8**

**9:30 - 10:00 AM Room B December 19**

**B24: Plasmonic semiconductors for photothermal therapy in the NIR-II window**

Jiang Jiang\*

*Suzhou Institute of Nano-tech and Nano-bionics, Chinese Academy of Sciences, China*

\*Corresponding author. Email: [jjiang2010@sinano.ac.cn](mailto:jjiang2010@sinano.ac.cn)

**Abstract**

Self-doped copper chalcogenide nanocrystals show broad plasmonic resonances covering NIR-II window [1], where optical transmission through tissue is optimal and higher maximum permissible exposure to laser irradiation is allowed. They are strong candidates for photothermal theranostic applications. By developing a facile aqueous phase synthetic route, monodisperse  $\text{Cu}_{2-x}\text{Se}$  nanocrystals with controlled size and surface properties have been prepared [2], and their plasmonic absorption was found to depend strongly on the physicochemical attributes. Through size and surface optimizations, these  $\text{Cu}_{2-x}\text{Se}$  nanocrystals have been applied to photoacoustic imaging guided photothermal therapy, along with their cytotoxicity and blood circulation properties investigated. Furthermore, through an in situ deposition of a thin  $\text{MnO}_2$  shell on  $\text{Cu}_{2-x}\text{Se}$ , they display enhanced MRI signal in response to acidic pH,  $\text{H}_2\text{O}_2$ , and reducing environment, without compromising photothermal property of the inner  $\text{Cu}_{2-x}\text{Se}$  core [3]. This serves as a new method of constructing photothermal theranostic probes with tumor microenvironment responsive light-up MRI contrast enhancing capability.

**Keywords**

copper chalcogenide; theranostic; NIR-II; photothermal; photoacoustic imaging

**References**

- [1] J. M. Luther, P. K. Jain, T. Ewers, A. P. Alivisatos, Localized Surface Plasmon Resonances Arising from Free Carriers in Doped Quantum Dots. *Nat. Mater.* 10, 361 (2011). doi: 10.1038/nmat3004
- [2] X. Ding, D. Fu, Y. Kuang, Y. Zou, X. Yang, L. Feng, X. Sun, H. Wu, J. Jiang, Seeded Growth of  $\text{Cu}_{2-x}\text{Se}$  Nanocrystals and Their Size-Dependent Phototherapeutic Effect. *ACS Appl. Nano Mater.* 1, 3303 (2018). doi: 10.1021/acsanm.8b00516
- [3] D. Fu, X. Ding, J. Wu, C. Li, Q. Wang, J. Jiang, Cationic Polyelectrolyte Mediated Synthesis of  $\text{MnO}_2$ -Based Core-Shell Structures as Activatable MRI Theranostic Platform for Tumor Cell Ablation. *Part. Part. Syst. Charact.* 35, 1800078 (2018). doi: 10.1002/ppsc.201800078



Session B8

10:00 - 10:30 AM Room B December 19

## B25: Janus Drug-Drug Conjugate Nanocapsules for enhancing Cancer Therapeutic Efficacy

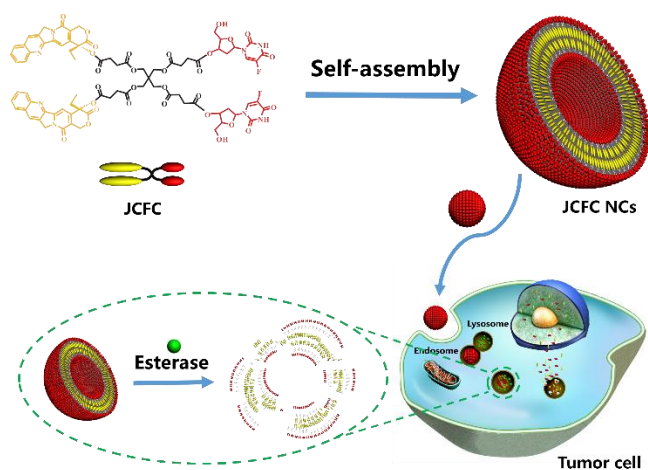
Zhifei Dai\*

Department of Biomedical Engineering, College of Engineering, Peking University, China

\*Corresponding author. Email: zhifei.dai@pku.edu.cn

### Abstract

A novel uniform liposome-like nanocapsule (NCs) was self-assembled for the first time from an amphiphilic Janus camptothecin-floxuridine conjugate (JCFC). JCFC NCs represent a strategy to deliver and preserve a fixed 1:1 molar ratio of the two drugs in a liposomal manner that can suppress premature burst release and coordinate the pharmacokinetics of the different drugs after i.v. administration. Our results demonstrate that the long blood retention time of the JCFC NCs facilitates the high tumorous accumulation of anticancer drugs via EPR effect and the subsequent cellular internalization into tumor cells. Owing to the esterase and acid hydrolysis of the ester bond in tumor cells, both camptothecin and floxuridine can be coordinately released from the JCFC NCs, resulting in higher apoptotic rate and synergetic anticancer activity than the individual free drugs and the mixture of camptothecin and floxuridine. We believe that JCFC NCs will soon begin to reach their full potential as an important class of therapeutic liposomal formulations and will contribute to remarkable advances in cancer treatments due to their unique features including clever use of JCFC itself as active liposomal building units, significantly high drug loading content, highly stable co-delivery drug combinations compared with competing conventional liposomes.



**Scheme 1.** Self-assembly of Janus camptothecin-floxuridine conjugate into the liposome-like nanocapsule for cancer combination therapy.

**Related Recent Publications**

- [1] Liang X, Gao G, Cui L, Wang S, Wang J, Dai Z(2018) Self-assembly of Amphiphilic Janus Camptothecin-Floxuridine Conjugate into Liposome-like Nanocapsules for More Efficacious Combination Chemotherapy in Cancer. *Adv Mater* 1703135
- [2] Liang X, Xu Y, Gao G, Zhou Y, Zhang N, Dai Z(2018) Ultrasound contrast agent microbubbles with ultrahigh loading capacity of camptothecin and floxuridine for enhancing tumor accumulation and combined chemotherapeutic efficacy. *NPG Asia Mater*, in press
- [3] Chen M, Liang X, Gao G, Zhao R, Zhang N, Wang S, Chen W, Zhao B, Wang J, Dai Z(2018) Ultrasound Triggered Conversion of Porphyrin/Camptothecin-Fluoroxuridine Triad Microbubbles into Nanoparticles Overcomes Multidrug Resistance in Colorectal Cancer. *ACS Nano* 2018, 12 (7), 7312–7326
- [4] Xu Y, Liang X, Bhattarai P, Sun Y, Zhou Y, Wang W, Chen W, Ge H, Wang J, Cui L, Dai Z (2017) Enhancing therapeutic efficacy of combined cancer phototherapy by ultrasound-mediated in situ conversion of near-infrared cyanine/porphyrin microbubbles into nanoparticles. *Adv Funct Mater* 1704096

**Session B9**

**11:00 - 11:30 AM Room B December 19**

**B26: Formation of micro/nano wrinkles on polymeric surfaces**

Dae Kun Hwang<sup>1,2,3,\*</sup>

<sup>1</sup>*Department of Chemical Engineering, Ryerson University, 350 Victoria Street, Toronto, Ontario, M5B 2K3, Canada*

<sup>2</sup>*Keenan Research Centre for Biomedical Science, St. Michael's Hospital, 30 Bond Street, Toronto, Ontario, M5B 1W8, Canada*

<sup>3</sup>*Institute for Biomedical Engineering, Science and Technology (iBEST), a partnership between Ryerson University and St. Michael's Hospital, 30 Bond Street, Toronto, Ontario, M5B 1W8, Canada*

\*Corresponding author. Email: dkhwang@ryerson.ca

**Abstract**

Micro/nano wrinkled surfaces have excellent characteristics, such as significantly enlarged surface area and enhanced adhesion. These characteristics have recently used as surface platforms for many emerging applications in electrical, mechanical, and biological processes. In particular, nano-wrinkles offer additional physical features, such as superhydrophobicity and enhanced Raman scattering. Although several fabrication techniques have been successfully developed to generate wrinkles at micro/nano scales, they are mostly limited to simple planar surfaces. Creating controllable multiscale wrinkles on multi-planar surfaces has remained challenging. We develop a simple pathway to form spatially tunable wrinkles at micro/nano scales on non-planar polymeric surfaces. In this texturing method, we make PEG (polyethylene glycol) microstructures, for instance, microposts using non-uniform photopolymerization in a PDMS channel. After a controllable washing step to remove the excess unpolymerized PEG, the partially cured top layer spontaneously forms wrinkles upon plasma treatment. We can simply control wrinkle wavelength by controlling the thickness of the partially cured top-layer.

**Session B9**

**11:30 - 12:00 PM Room B December 19**

## **B27: A Novel “Micro-capillary ELISA” for Detecting Salivary Biomarkers**

### **Aiming for POC Applications**

Wan-Joong Kim<sup>1,2</sup>, Young Jun Kim<sup>1,\*</sup>

<sup>1</sup>Biohealth IT Convergence Technology Research Department, Electronics and Telecommunications Research Institute, Daejeon 34129, Republic of Korea

<sup>2</sup>Biosensor Research Group, DMX Corporation, 1184, Yuseong-gu, Daejeon, 34109, Republic of Korea

\*Corresponding author. Email: junkim@etri.re.kr

#### **Abstract**

We developed a novel immunoassay system in a micro-scale capillary tube aiming to apply for point-of care environment. In particular the “ $\mu$ -capillary ELISA” was designed to detect stress biomarkers in saliva. C-reactive protein (CRP) and cortisol had been reported to be related with psychological stress, and also are secreted in saliva [1-2]. Conventionally measuring the level of cortisol necessitates a tedious collection process in which a person is required to spend a whole in a hospital to amass urine sample. The concentration of CRP and cortisol is decided by ELISA which is composed of multi-steps and processed by an experienced personnel. However use of “ $\mu$ -capillary ELISA” in assaying the stress biomarkers in saliva not only simplifies the assay process but also has added advantage of being a non-invasiveness.

Surface chemistry is one the major factors that decides the performance of the “ $\mu$ -capillary ELISA”. We developed a vapor-phase surface modification in immobilizing aminopropyl triethoxysilane (APTES). The efficiency of the vapor-phase amination was confirmed by comparing with that of the solution method through attaching gold nanoparticles on the two amine surfaces. Using the “ $\mu$ -capillary ELISA” prepared via vapor-phase amination, at least 0.1 ng/mL of CRP could be detected [3]. In devising a “ $\mu$ -capillary ELISA” for cortisol, in order to overcome problems caused by the small molecular weight of cortisol, four different types of surface chemistries for competitive immunoassays were compared. Choosing the best resulting process in which cortisol was immobilized with (3-trimethoxysilylpropyl) diethylenetriamine (TMPED), the “ $\mu$ -capillary ELISA” system could detect cortisol as low as 50 pg/mL in artificial saliva. Also we developed a nanoparticle system to enhance detection performance in “ $\mu$ -capillary ELISA” [4].

In conclusion, use of the novel “ $\mu$ -capillary ELISA” system in detecting salivary biomarkers, together with added technical development in surface chemistry and nanoparticles, is likely to make useful applications in POC environments. The future research is focused on installing the “ $\mu$ -capillary ELISA” system to hand-held sensors equipped to wirelessly communicate with a mobile-phone.

#### **Keywords**

Micro-capillary; immunoassay; saliva; stress biomarkers and nanoparticles

#### **References**

- [1] M. K. Wium-Andersen; D. D. Ørested; S. F. Nielsen; B. G. Nordestgaard, Elevated C-Reactive Protein Levels, Psychological Distress and Depression in 73131 Individuals, *Jama Psychiatry* 70, 176 (2013). doi: 10.1001/2013.jamapsychiatry.102
- [2] D. H. Hellhammer; S. Wust; B. M. Kudielka, Salivary Cortisol As a Biomarker in Stress Research, *Psychoneuroendocrinology*. 34, 163 (2009) doi:10.1016/j.psyneuen.2008.10.026
- [3] W.-J. Kim, S. H. Hyun, H. Y. Cho, S. Byun, B. K. Kim, C. Huh, K. H. Chung, Y. J. Kim, Sensitive “capillary ELISA” via vapor-phase surface modification, *Sensors and Actuators B* 233, 281 (2016) doi:10.1016/j.snb.2016.04.072
- [4] W.-J. Kim, H. Y. Cho, B. Jeong, S. Byun, J.D. Huh, Y. J. Kim, Synergistic Use of Gold Nanoparticles (AuNPs) and “Capillary Enzyme-Linked Immunosorbent Assay (ELISA)” for High Sensitivity and Fast Assays, *Sensors* 18, 55 (2018), doi:10.3390/s18010055

**Session B9**

**12:00 - 12:30 PM Room B December 19**

## **B28: Surface Modification of ZnO Nanoparticles by Core-Shell**

### **Nanoparticles Decreased Cytotoxicity towards HeLa Cancer Cells: A facile Approach for Safer Nanomaterials**

Amna Sirelkhatim<sup>1,\*</sup>, Shahrom Mahmud<sup>2</sup>, Azman Seen<sup>3</sup>, Noor Haida Mohd Kaus<sup>4</sup>

<sup>1</sup>*Physics section, Department of Science, Faculty of Education, Sudan University of Science and Technology (SUST), Khartoum, Sudan*

<sup>2</sup>*Institute of Nano-Optoelectronics Research and Technology (INOR), School of Physics, Universiti Sains Malaysia (USM), 11800 Minden, Pulau Pinang, Malaysia*

<sup>3</sup>*Advanced Medical and Dental Institute, Cluster of Integrative Medicine, Universiti Sains Malaysia (USM), 13200, Bertam, & IPHarm, NIBM, Malaysia*

<sup>4</sup>*School of Chemical Sciences, Universiti Sains Malaysia (USM), 11800 Minden, Pulau Pinang, Malaysia*

\*Corresponding author. Email: amnasirelkhatim@yahoo.co.uk

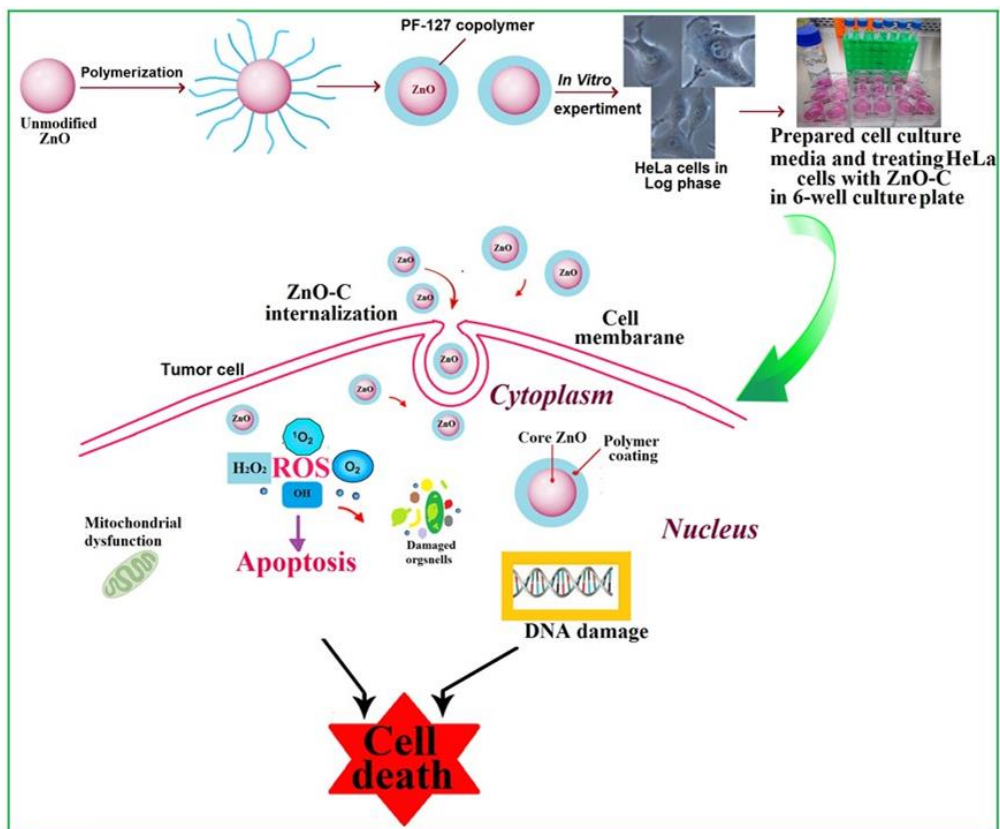
#### **Abstract**

This study was designed to develop an effective strategy of a core-shell nanoparticle structure as a distinctive formula to achieve decreased toxicity of nanomaterials. The structure was fabricated through surface modification by introducing Pluronic F-127 copolymer (PF-127) as a shell coating ZnO nanoparticle (ZnO-NPs) core. Employing a simple solution process. Two equally sized ZnO-NPs samples were synthesized, the stabilized coated ZnO-C (representing the core/shell), and the as-purchased sample ZnO-A. The cytotoxicity was studied on the human cervix cancer cells (HeLa) and was much reduced by ZnO-C, whereas its unique properties were preservative, as evidential by the structural and morphological investigations through XRD, TEM, and FESEM. These characterizations revealed similarities in crystal structure, high purity, identical morphologies and average cores sizes (60nm) in the two samples. Conversely, FTIR spectroscopy exhibited significant dissimilarities in their surface chemistry showing varied surface functional groups. Subsequently, zeta potential measurements as well showed big differences in their surface charges (36.3mV and 24.3mV). Importantly, these improvements in the physiochemical properties resulted in major differences in their cytotoxicity to HeLa cells, which is a vital aim of this study. The obtained IC<sub>50</sub> values 25mM by ZnO-C and 0.2mM by ZnO-A, indicated selective reliable doses and biocompatibility due to ZnO-C colloidal stability that led to a controlled release into HeLa cells and prolonged action. Therefore, the cytotoxicity was definitely tailored. Additionally, trypan blue exclusion assay (TBEA), showed a dose-dependent fashion cytotoxic effects that ZnO-A effectively reduced HeLa cell viability (37%, and 18.4%, at 0.25 and 0.35mM respectively), while ZnO-C exhibited higher cell viability (94% and 79% at 15 and 20mM respectively). Furthermore, reactive oxygen species (ROS) were much generated by ZnO-A (45%) than ZnO-C (30%) and induced higher apoptosis (49.70%, 40.20% respectively) indicative by the morphological changes (FESEM images) visualized by microscopic means. Moreover, the toxicity was found to depend on the coating level, more PF-127 coating layers caused substantial decrease in ZnO-NPs toxicity. Based on these findings, ZnO-NPs in such a core-shell design can be a promising approach presenting a safer nanomaterial in biomedical applications as well as in other industries.

**Keywords**

ZnO nanoparticles; Core/shell Nanoparticles; Pluronic F-127 copolymer; Surface modification; HeLa cancer cells; Toxicity

**Graphical abstract**



**Session B10**

**14:00 - 14:30 PM Room B December 19**

**B29: Shape memory fibrous scaffolds for bone tissue engineering**

Yanzhong Zhang<sup>1,2,3,\*</sup>

<sup>1</sup>College of Chemistry, Chemical Engineering & Biotechnology, Donghua University, 2999 North Renmin Road, Shanghai 201620, China

<sup>2</sup>State Key Laboratory for Modification of Chemical Fibers & Polymer Materials, Donghua University, 2999 North Renmin Road, Shanghai 201620, China

<sup>3</sup>Key Lab of Science & Technology of Eco-Textile, Ministry of Education, Donghua University, 2999 North Renmin Road, Shanghai 201620, China

\*Corresponding author. Email: yzzhang@dhu.edu.cn

**Abstract**

In bone tissue engineering, a significant challenge remains in the design and fabrication of ideal biomaterial scaffolds that are capable of recapitulating the cellular microenvironments, both biologically and biomechanically. While electrospinning has been well-documented for enabling to biomimetically construct the cell-residing extracellular matrix, how to exert in situ mechanical stimuli upon post-implantation of the scaffolds is an issue to be addressed. Having the biodegradable scaffolds integrated with shape memory functionality [1] may offer a solution to this problem. This presentation gives a brief overview of our recent works [2-4] in developing electrospun biomimicking fibrous scaffolds with shape memory effects for potential use towards in situ bone regeneration. We demonstrated that shape memory capable scaffolds hold a great potential in achieving enhanced efficacy in physiologically repairing various bone defects with the bone tissue engineering approach.

**Keywords**

Shape memory effects; Electrospinning; Fibrous scaffolds; Bone tissue engineering

**References**

- [1] M. Bao; Q.H. Zhou; W. Dong; X.X. Lou; Y.Z. Zhang, Ultrasound-Modulated Shape Memory and Payload Release Effects in a Biodegradable Cylindrical Rod Made of Chitosan-Functionalized PLGA Microspheres. *Biomacromolecules*. 14, 1971 (2013). doi: 10.1021/bm4003464
- [2] M. Bao; X.X. Lou; Q.H. Zhou; W. Dong; H.H. Yuan; Y.Z. Zhang, Electrospun Biomimetic Fibrous Scaffold from Shape Memory Polymer of PDLLA-co-TMC for Bone Tissue Engineering. *ACS Applied Materials & Interfaces*. 6, 2611 (2014). doi: 10.1021/am405101k
- [3] M. Bao; X.L. Wang; H.H. Yuan; X.X. Lou, Q.H. Zhao; Y.Z. Zhang, HAp Incorporated Ultrafine Polymeric Fibers with Shape Memory Effect for Potential Use in Bone Screw Hole Healing. *Journal of Materials Chemistry B*. 4, 5308 (2016). doi: 10.1039/c6tb01305h
- [4] Y. Zhou; X.L. Wang; B.C. Yi; Z.P. Yu; S.Y. Yang; Y.B. Shen; Y.Z. Zhang, Engineering Shape Memory Enabled Composite Nanofibers for Bone Tissue Engineering. *Chemical Journal of Chinese Universities-Chinese*. 39, 1554 (2018). doi: 10.7503/cjcu20170838

**Session B10**

**14:30 - 15:00 PM Room B December 19**

**B30: Capped gold and silver clusters as efficient contrast agents for bio-imaging? Exploring new routes to enhance their emission properties**

Rodolphe Antoine\*

*Univ Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, UMR 5306 F-69622, Lyon, France*

\*Corresponding author. Email: rodolphe.antoine@univ-lyon1.fr

**Abstract**

Functional ligand-protected noble metal cluster nanomaterials [1] with enhanced two-photon absorption and two-photon excited emission may lead to new technologies in the fields of bio-imaging applications. In this contribution, I will review experimental and theoretical methodologies allowing detailed investigation and analysis of two-photon absorption/emission properties of ligand-protected silver and gold metal clusters, coined “ligand-core” NLO-phores. [2, 3] Then I will thoroughly analyze physical phenomena and trends leading to large two-photon absorption/emission responses of a few series of model nanoclusters [4, 5] focusing on the effects of the relaxation pathways in the linear and nonlinear optical regime, as well as innovative strategies aiming at enhancing their two-photon emission responses. [6-8]

**References**

- [1] R. Antoine and V. Bonačić-Koutecký, *Liganded silver and gold quantum clusters. Towards a new class of nonlinear optical nanomaterials*, Springer International Publishing, 2018
- [2] Russier-Antoine I, Bertorelle F, Calin N, Sanader Z, Krstic M, Comby-Zerbino C, et al. Ligand-core NLO-phores: a combined experimental and theoretical approach to the two-photon absorption and two-photon excited emission properties of small-ligated silver nanoclusters. *Nanoscale*. 2017;9(3):1221-28
- [3] Sanader Z, Krstic M, Russier-Antoine I, Bertorelle F, Dugourd P, Brevet P-F, et al. Two-photon absorption of ligand-protected Ag<sub>15</sub> nanoclusters. Towards a new class of nonlinear optics nanomaterials. *Physical Chemistry Chemical Physics*. 2016;18:12404-08
- [4] Bertorelle F, Russier-Antoine I, Calin N, Comby-Zerbino C, Bensalah-Ledoux A, Guy S, et al. Au<sub>10</sub>(SG)<sub>10</sub>: A Chiral Gold Catenane Nanocluster with Zero Confined Electrons. *Optical Properties and First-Principles Theoretical Analysis*. *The Journal of Physical Chemistry Letters*. 2017;8(9):1979-85
- [5] Russier-Antoine I, Bertorelle F, Hamouda R, Rayane D, Dugourd P, Sanader Z, et al. Tuning Ag<sub>29</sub> nanocluster light emission from red to blue with one and two-photon excitation. *Nanoscale*. 2016;8(5):2892-98
- [6] Bertorelle F, Moulin C, Soleilhac A, Comby-Zerbino C, Dugourd P, Russier-Antoine I, et al. Bulky counterions: enhancing the two-photon excited fluorescence of gold nanoclusters. *ChemPhysChem*. 2018;19:165-68
- [7] Shen D, Henry M, Trouillet V, Comby-Zerbino C, Bertorelle F, Sancey L, et al. Zwitterion functionalized gold nanoclusters for multimodal near infrared fluorescence and photoacoustic imaging. *APL Materials*. 2017;5(5):053404
- [8] Waszkielewicz M, Olesiak-Banska J, Comby-Zerbino C, Bertorelle F, Dagany X, Bansal AK, et al. pH-Induced transformation of ligated Au<sub>25</sub> to brighter Au<sub>23</sub> nanoclusters. *Nanoscale*. 2018;10(24):11335-41



**Session B10**

**15:00 - 15:30 PM Room B December 19**

## **B31: Peptide-Modified PLL-coated Aligned PEDOT:PSS Fibers Promotes the Growth of PC12-derived Nerve Cells**

Jiashing Yu\*, Raymond Christopher Setiawan, Ruiken Sim

*Dept. of Chemical Engineering, National Taiwan University, Taipei*

\*Corresponding author. Email: jiayu@ntu.edu.tw

### **Abstract**

Preceding researches have shown that PC12-derived neural cells cultivated on aligned PEDOT:PSS fibers show a longer neurite outgrowth and increased neural-markers gene expression upon electrostimulation [1]. However, the resulting cell viability of such treatment is considerably lower when compared to the control group cultivated on TCPS. In this experiment, we try to investigate the possibility of adhering anionic laminin-derived peptide (DCDEGYIGSR) on the electrospun material so as to increase both of the cell viability and corresponding gene expression of the said neural cells [2].

Poly-L-Lactide has been shown to be a good candidate as a bio-linker [3]. Upon contact with PLL solution, PEDOT:PSS will adsorb the polymers onto its surface. The peptides will be attached by means of EDC/NHS coupling. The modified surface will be tested for its hydrophilicity (contact angle), surface morphology (AFM and SEM) and its surface energy (XPS). Fluorescamine staining will be conducted on PLL coated PEDOT:PSS. BCA Assay will be conducted as to determine the grafting ratio of the peptide onto the surface.

After the electrostimulation, the cell culture will be assessed for its growth characteristics. Alamar Blue staining will be used to determine its cell metabolism rate curve for the selected time points. Live and Dead staining will also be carried out at the end of the culture. RT-PCR will be conducted on Nestin, Tuj-1 and MAP2 gene to reveal the cell's gene expression for the groups with and without peptide modification. Immunostaining on Nestin and Tuj-1 will be conducted and confocal imagery will then be obtained so as to visualize the resulting culture of its neurite outgrowth and cell morphology.

Generally, this shows that our effort may be promising and particularly a novel work in this scope, since there has been no study conducted on how to make an aligned PEDOT:PSS fiber and have its surface modified at the same time. Furthermore, such study may give a good insight on how the effect of these two variables interact with each other and how they may be concerted together so as to bring out a better method to be further applied in clinical settings.

### **Keywords**

Aligned nanofibers; surface modification; functionalization of peptides; PEDOT; PSS; PLL

### **References**

- [1] Chang YJ, Hsu CM, Lu MS, Chen L. Electrical Stimulation Promotes Nerve Growth-Factor Induced Neurite Outgrowth and Signalling. *Biochim Biophys Acta*. 1830(8):4130-6 (2013). doi: 10.1016/j.bbagen.2013.04.007
- [2] Green, et.al. Cell Attachment Functionality of Bioactive Conductive Polymers for Neural Interfaces. *Biomaterials* 30 (2009):3637-3644. doi: 10.1016/j.biomaterials.2009.03.043
- [3] Yu J, et.al. Electrospun PLGA Fibers Incorporated with Functionalized Biomolecules for Cardiac Tissue Engineering. *Tissue Engineering* 20 (2014):1896-1907. doi: 10.1089/ten.TEA.2013.0008

**Session B11**

**16:00 - 16:30 PM Room B December 19**

**B32: Bio-Hybrid Hydrogel Comprising Animal and Plant Sources**

**Embedded with Protein Capped Silver Nanoparticles for Accelerated Tissue Regeneration in Chronic Tissue Defects**

Ragothaman Murali<sup>1,2</sup>, Palanisamy Thanikaivelan<sup>1,\*</sup>

<sup>1</sup>*Advanced Materials Laboratory, Central Leather Research Institute (Council of Scientific and Industrial Research), Adyar, Chennai 600020, India*

<sup>2</sup>*Centre for Biotechnology, Anna University, Chennai 600025, India*

\*Corresponding author. Email: thanik8@yahoo.com

**Abstract**

The clinical management of a variety of tissue defects resulting from a traumatic insult (superficial and chronic wounds), oncological resection or progressively degenerative diseases (such as diabetic foot ulcer and many others), is a formidable challenge to the current standard of treatment aiming at structural and functional reconstruction. Hydrogel-based drug delivery system has emerged as a promising platform for chronic tissue defects due to their inherent ability to facilitate the moist microenvironment with better biocompatibility and accelerated tissue regeneration. Here, we have synthesized the aminated xanthan gum and the biomimetic silver nanoparticles by treating the xanthan gum with ethylene diamine and by employing the aqueous collagen as a reducing and stabilizing agent, respectively. We have also developed a stable bio-hybrid hydrogel system comprising of collagen (C) as a biocompatible polymer, aminated xanthan gum (AXG) as a biodegradable polymer and gelling agent, biomimetic silver nanoparticles (AGNP) as an antimicrobial agent and melatonin (MELT) as an antioxidant and anti-inflammatory agent. The prepared C-AXG-AGNP-MELT hydrogel system exhibits better gelation, surface morphology, rheology and degelation properties. In vitro antibacterial studies demonstrate that the C-AXG-AGNP-MELT hydrogel system remarkably inhibited both gram-positive and gram-negative bacterias namely *Bacillus subtilis*, *Staphylococcus aureus*, *Escherichia coli* and *Pseudomonas aeruginosa*. The in vitro cell culture assessment of the prepared hydrogel system showed excellent biocompatibility when cultured with the NIH 3T3 fibroblast cell lines. We also evaluated the wound healing efficiency of the prepared C-AXG-AGNP-MELT hydrogel system in a full-thickness open excisional skin wound model in Wistar albino rats. The results indicate that the application of C-AXG-AGNP-MELT hydrogel system enhances re-epithelialization of epidermis and collagen deposition in the wound tissue owing to its excellent antimicrobial, antioxidant and anti-inflammatory properties. Our findings suggest that the developed C-AXG-AGNP-MELT hydrogel system can be used as a promising wound dressing material for treating infected burn and chronic tissue defects.

**Keywords**

Collagen; Silver Nanoparticles; Aminated Xanthan Gum; Antimicrobial; Tissue Regeneration; Wound Healing

**Session B11**

**16:30 - 17:00 PM Room B December 19**

## **B33: Multifunctional Plasmonic and Luminescent Nanomaterials for Smart Biosensors and Theranostics Applications**

Yen Nee Tan<sup>1,2,\*</sup>, Yong Yu<sup>2</sup>, Xinting Zheng<sup>2</sup>, Victor Xu<sup>2</sup>

<sup>1</sup>Newcastle University, 537 Clementi Road, SIT@NP Building, Singapore

<sup>2</sup>Institute of Materials Research and Engineering, 2 Fusionopolis Way, Singapore

\*Corresponding author. Email: yennee.tan@newcastle.ac.uk

### **Abstract**

Inspired by Natural biomineralization processes in creating functional nanostructured materials under benign conditions from the bottom up, our research focuses on the development of biogenic nanomaterials for a vast plethora of biomedical applications. Firstly, I will talk about the rational design of peptide- and nucleic acid-based biomolecular templates for the synthesis of multifunctional metallic and carbon-based nanoparticles with tunable optical properties (i.e., plasmon absorption and light emission) and biofunctionalities for sensing, imaging, delivery and therapy [1-9]. For example, we have designed self-assembly DNA templates to form redox-responsive silver nanoclusters (NCs < 2 nm in size) for two-way color change detection of free radicals and antioxidants in real time. Using bi-functional peptide templates, AuNCs with tunable emission color from visible to near-infrared wavelength have been successfully synthesized for targeted gene delivery and bioimaging applications [5]. We have also employed this bioinspired approach to ‘turn’ the native protein into bioactive fluorescent sensors for small molecule drug screening [6] and photodynamic therapy [7]. More recently, we have uncovered the first design principles of amino acid-derived photoluminescent bio-dots with tailored-made structure-properties to improve their photostability, intracellular uptake capability and biocompatibility [8]. Inspired by the natural antimicrobial peptides, benign antimicrobial biodot that possesses both the unique photochemical properties of nanoparticles and biomaterials has been developed for combating broad spectrum multi-drug resistant bacteria [9]. The second part of my presentation will focus on the bio-functionalization strategies of noble metal nanoparticle for biosensor development, which can convert the ‘invisible’ biological responses into easily measurable and observable colorimetric outputs [10,11]. By exploiting the plasmonic coupling, fluorescence and/or light scattering properties of the nanometals, we have developed a series of label-free nanosensors to detect a wide range of bio-analytes such as drugs, biomarkers, pathogens, etc., and for studying important biomolecular interactions such as gene transcription, DNA mutation and enzymatic reaction [12-16]. These bioassays are versatile, efficient and low-cost with high throughput sensing capability. These smart nanobiosensors are versatile, efficient and low-cost, which could culminate into tangible products useful for biomedical research and diagnostics. The fundamental understanding on the intertwined relationships of biological processes and nanochemistry can contribute on tailoring multifunctional biocompatible and smart nanomaterials towards theranostics and personalized medicine in the future.

### **Keywords**

Bioinspired Synthesis; Plasmonic nanoparticles; Photoluminescence; Biosensor; Nanomedicine

### **References**

- [1] X. T. Zheng; V. H. Xu; Y. N. Tan\*, *Bioinspired Design and Engineering of Functional Nanostructured Materials*. *Advances in Bioinspired and Biomedical Materials Vol. 2*, American Chemical Society (ACS) Book, 1253, 123-152 (2017)
- [2] Y. Yu; B. Y.L. Mok; X.J. Loh; Y. N. Tan\*, *Rational Design of Biomolecular Templates for Synthesizing Multifunctional Noble Metal Nanoclusters towards Personalized Theranostic Applications*. *Advanced Healthcare Materials* (2016). DOI: 10.1002/adhm.201600192
- [3] V. H. Xu; X. T. Zheng; B. Y.L. Mok; S.A. Ibrahim; Y. Yu; Y. N. Tan\*, *Molecular Design of Bioinspired Nanostructures for Biomedical Applications: Synthesis, Self-Assembly and Functional Properties.* *Journal of Molecular and Engineering Materials*, 04, 1640003-1640036 (2016)
- [4] Y. N. Tan; J. Y. Lee; Daniel. I. C. Wang\*, *Uncovering the Design Rules for Peptide Synthesis of Metal Nanoparticles*. *Journal of American Chemical Society*, 132, 5677-5686 (2010)
- [5] Y. Yu; J. C. Yi; Y. N. Tan\*, *Microwave-Assisted Synthesis and Mechanistic Study of Multicolor Emissive Au Nanoclusters using Thiol-Containing Biomolecules*. *Adv. Mater. Lett.* 9 (9), 647-651(2018).
- [6] Y. Yu; S. Y. New; J. Xie; X. Su; Y. N. Tan\*, *Protein-Based Fluorescent Metal Nanoclusters for Small Molecular Drug Screening*. *Chemical Communications*, 50, 13805-13808 (2014).
- [7] Y. Yu; J. Geng; E.X.O, Yong; V. Chellappan; Y. N. Tan\*, *Bovine Serum Albumin Protein-Templated Silver Nanocluster (BSA-Ag13): An Effective Singlet Oxygen Generator for Photodynamic Cancer Therapy*”, *Advanced Healthcare Materials*. (2016). DOI:10.1002/adhm.201600312.
- [8] H.V. Xu; X. T. Zheng; Y. Zhao; Y. N. Tan \*, *Uncovering the Design Principle of Amino Acid-Derived Photoluminescent Biodots with Tailor-Made Structure–Properties and Applications for Cellular Bioimaging.* *ACS Applied Materials and Interfaces*, 10, 19881–19888 (2018).
- [9] H.V. Xu; X. T. Zheng; C. Wang; Y. Zhao; Y. N. Tan\*, *Bioinspired Antimicrobial Nanodots with Amphiphilic and Zwitterionic-like Characteristics for Combating Multidrug-Resistant Bacteria and Biofilm Removal.* *ACS Applied Nano Materials* 1, 2062–2068 (2018).
- [10] W. L. P. Goh; J. F. Ghadessey; D. P. Lane; X. T. Zheng; E. Assah; Y. N. Tan\*, *Transcription Factors As Detection And Diagnostic Biomarkers In Cancer*. *Next Generation Point-Of-Care Biomedical Sensors Technologies for Cancer Diagnosis*. Springer Nature Book, DOI: 10.1007/978-981-10-4726-8 (2017).
- [11] Y. N. Tan\*; X. T. Zheng; Y. Yu, *Metallic Nanobiosensor for Biological Analysis and Medical Diagnostics*. *Nanobiosensors for Personalized and Onsite Biomedical Diagnostics*. The Institution of Engineering and Technology Book, 537-559 (2015).
- [12] J. Song; Y. N. Tan\*; D. Jańczewski; M. A. Hempenius; J. W. Xu; H. R. Tan; G. J. Vancso\*, *Poly(ferrocenylsilane) Electrolytes as Gold Nanoparticle Foundry: Two-in-One Redox Synthesis, Electrosteric Stabilization, and Sensing Applications*”, *Nanoscale* DOI: 10.1039/C7NR04697A (2017)
- [13] E. Assah; W. L. P. Goh; X. T. Zheng; D. P. Lane; J. Li; T. X. Lim; J. F. Ghadessey; Y. N. Tan\*, *Rapid Colorimetric Detection Of P53 Protein Function Using DNA-Gold Nanoconjugates with Applications For Drug Discovery and Cancer Diagnostics*. *Colloids and Surfaces B: Biointerfaces*, 169, 214-221(2018), DOI.org/10.1016/j.colsurfb.2018.05.007
- [14] X. T. Zheng; W. L. P. Goh; P. Yeow; D. P. Lane; J. F. Ghadessey; Y. N. Tan\*, *Ultrasensitive Dynamic Light Scattering Based Nanobiosensor For Rapid Anticancer Drug Screening*. *Sensors and Actuators B: Chemical*, 279, 79-86 (2018). Doi.org/10.1016/j.snb.2018.09.088
- [15] N. J. Seow; Y. N. Tan\*; X. Su; Lanry Yung\*, *DNA-Directed Assembly of Nanogold Dimers: A Unique Dynamic Light Scattering Sensing Probe for Transcription Factor Detection*, *Scientific Report*, 5:18293 (2015). DOI: 10.1038/srep18293.
- [16] Y. N. Tan; X. Su; Y. Zhu; J. Y. Lee, *Sensing Of Transcription Factor Through Controlled-Assembly of Metal Nanoparticles Modified With Segmented DNA Elements*. *ACS Nano*, 4, 5101–5110 (2010)

**Session B11**

**17:00 - 17:30 PM Room B December 19**

**B34: T1/T2 Dual functional iron oxide MRI contrast agent with super stability and low hypersensitivity**

Chongchong Miao<sup>1</sup>, Fenglin Hu<sup>1</sup>, Yuanpeng Rui<sup>2</sup>, Yourong Duan<sup>3</sup>, Hongchen Gu<sup>1,\*</sup>

<sup>1</sup>Nano Biomedical Research Center, School of Biomedical Engineering & Med-X Research Institute, Shanghai Jiao Tong University, 1954 Huashan Road, Shanghai, 200030, China

<sup>2</sup>Department of Radiology, Putuo Hospital, Shanghai University of Traditional Chinese Medicine, Shanghai 200062, China

<sup>3</sup>State Key Laboratory of Oncogenes and Related Genes, Shanghai Cancer Institute, Renji Hospital, School of Medicine, Shanghai Jiao Tong University, Shanghai 200032, China

\*Corresponding author. Email: hcgu@sjtu.edu.cn

**Abstract**

Clinical acceptable safety and efficacy are the most important issues for the design and synthesis of iron oxide MRI contrast agent. To meet the requirements we developed a kind of low molecular weight PAA-coated Fe<sub>3</sub>O<sub>4</sub> nanoparticles (CS015) with super colloidal stability and low hypersensitivity benefited by ultrahigh carboxyl group density. The constitution and physicochemical properties of the particles were characterized by TEM, XRD, FTIR and TGA. Ultrahigh density of COOH on the particles (33 COOH/nm<sup>2</sup>) was verified while core size (5.1 nm) and dynamic diameter (41 nm) with narrow distribution were also achieved. The particles showed excellent dispersity and stability even after re-dissolving spray-dried and freeze-dried samples, at high temperature sterilized conditions and long-term storage. The nanoparticles could quickly capture iron ions in bulk solution from ITC results and bioactive iron of CS015 was greatly decreased (0.54±0.05 mg/L) compared to commercial available Ferumoxytol, Iron Sucrose and VSOP. Free iron ions release was 1120 times lower than iron toxic concentration. An excellent low cytotoxicity and less risk of hypersensitivity of CS015 had been manifested by cytotoxicity experiments and passive cutaneous anaphylaxis test. T1 and T2-weighted MRI contrast effects both in vitro and in vivo had been verified made CS015 a potential dual MRI contrast agent. Theoretical calculated conformation was speculated and all the advantages mentioned above were benefited by the three dimensional brush-like texture of CS015. Therefore, these merits of CS015 exhibited great potential in MRI contrast agent for diagnostic applications.

**Keywords**

Superparamagnetic nanoparticles; MRI contrast agent; Stability; Hypersensitivity

**Session B11**

**17:30 - 18:00 PM Room B December 19**

## **B35: Nanotechnology and Environmental Application: Future with Electrospinning**

Shivendu Ranjan\*

*Faculty of Engineering and Built Environment, University of Johannesburg, Johannesburg, South Africa*

\*Corresponding author. Email: shivenduranjan@gmail.com

### **Abstract**

Nanotechnology is providing novel opportunities and solutions to guarantee sustainable energy and environments for the future. Materials of nanofiberous morphology are attractive to solve numerous energy and environmental issues. Nanofibers can be effectively produced by electrospinning, which is a simple and low cost technique. In addition, electrospinning allows the production of nanofibers from various materials e.g. organics and inorganics in different configurations and assemblies. The nanofibers used in filtration membranes for environmental remediation, minimize the pressure drop and provide better efficiency than conventional fiber mats. The large surface area-to-volume ratio of nanofiber membranes allows greater surface adsorption of contaminants from air and water, and increases the life-time of the filtration media. This review highlights the potential and application of electrospun nanofiberous materials for solving critical environmental issues. The main aim of this review will be to discuss the application of electrospun nanofibers for air and water filtration and to introduce the high-throughput electrospinning machine as well as the products for air and water filtration. This review will be equally important for scientists, professors, policy makers, industrialists and the students to understand the electrospinning process and its importance for environmental applications.

Overall the following will be discussed in this abstract:

- Reviews the recent advances in development of functional electrospun nano fibers
- Comprehensively introduces the environmental applications of electrospun nano fibers
- Provides a versatile strategy for design and development of functional nanomaterials towards environmental issues

### **Keywords**

Electrospinning; Environmental Nanotechnology; Ultra-filtration; Nanofibers; Air-filtration

### **Acknowledgment**

The authors would like to acknowledge E-Spin Nanotech Pvt Ltd for the funding support of the research project and providing the lab facilities. Authors would also like to acknowledge SIDBI Centre, IIT Kanpur for providing technical support to E-Spin Nanotech Pvt Ltd.

### **Reference**

- [1] Thavasi, V., Singh, G., Ramakrishna, S., Electrospun nanofibers in energy and environmental applications, *Energ. Environ. Sci.*, 1, 205-221, 2008
- [2] Deshpande, T. D., Yogesh R. G. S., Patil S., Sharma, A., To study surface and sub-surface nanomechanical properties of electrospun polyacrylonitrile (PAN) nanofibers/polydimethylsiloxane (PDMS) composites, *Soft Matter*. 14, 7829-7838, 2018

**Poster Session**

**Room C, December 18 2018**

## **P1: Dimension-dependent optoelectronic properties of perovskite-metal oxide core-shell nanocrystals**

Yunhee Cho<sup>1,2</sup>, Hyoyoung Lee<sup>1,2,3,\*</sup>

<sup>1</sup>Center for Integrated Nanostructure Physics (CINAP), Institute of Basic Science (IBS): 2066 Seoburo, Jangan-Gu, Suwon, Gyeonggi-Do 16419, Republic of Korea

<sup>2</sup>Department of Chemistry, Sungkyunkwan University: 2066 Seoburo, Jangan-Gu, Suwon, Gyeonggi-Do 16419, Republic of Korea

<sup>3</sup>Department of Energy Science, Sungkyunkwan University: 2066 Seoburo, Jangan-Gu, Suwon, Gyeonggi-Do 16419, Republic of Korea

\*Corresponding author. Email: hyoyoung@skku.edu

### **Abstract**

Recently, halide-perovskite materials are promising for various applications including optoelectronic devices such as solar cells, photodetectors and phototransistors due to their high absorption density, carrier diffusion length and easy solution process. [1-2] Thus, lots of methods have been developed to change the composition and morphology of the perovskite nanocrystals to modulate the optophysical properties. [3, 4] Especially, dimension of nanocrystals such as nanodots, nanorods, nanowires, nanosheets, and nanoplatelets confines the photogenerated charge carrier and change the charge transport performances.

However, the practical application of perovskite nanocrystals is still limited due to their unstability toward the oxygen, humidity, and light irradiation. Because the perovskite nanocrystals have the ionic properties and are passivated by labile ligands after solution synthesis via hydrogen bond. [5] Therefore, ligand exchange of synthesized nanocrystals into polymers and metal oxides, are suggested for the stability of perovskite nanocrystals. Titanium dioxide (TiO<sub>2</sub>), one of n-type metal oxide semiconductors, could protect the perovskite nanocrystals against environment and transfer the photogenerated electrons.

Here, we synthesize the perovskite nanocrystals with different dimension including 0D and 2D via hot injection methods and passivate the perovskite nanocrystals with TiO<sub>2</sub> to generate perovskite-metal oxide core-shell nanocomposite. The dimension-dependent optical and electrical properties of these nanocomposite are analyzed using HRTEM, XRD, UV-vis absorption and PL spectroscopy.

### **Keywords**

Perovskite nanocrystals; colloidal synthesis; core-shell; charge transfer

### **References**

- [1] Q.A. Akkerman, G. Rainò, M.V. Kovalenko, L. Manna, Genesis, challenges and opportunities for colloidal lead halide perovskite nanocrystals, *Nature Materials*, 17 (2018) 394-405
- [2] N.-G. Park, Perovskite solar cells: an emerging photovoltaic technology, *Materials Today*, 18 (2015) 65-72
- [3] S. Bai, Z. Yuan, F. Gao, Colloidal metal halide perovskite nanocrystals: synthesis, characterization, and applications, *Journal of Materials Chemistry C*, 4 (2016) 3898-3904
- [4] M.V. Kovalenko, L. Protesescu, M.I. Bodnarchuk, Properties and potential optoelectronic applications of lead halide perovskite nanocrystals, *Science*, 358 (2017) 745-750
- [5] H. Huang, M.I. Bodnarchuk, S.V. Kershaw, M.V. Kovalenko, A.L. Rogach, Lead Halide Perovskite Nanocrystals in the Research Spotlight: Stability and Defect Tolerance, *ACS Energy Letters*, 2 (2017) 2071-2083

**Poster Session**

**Room C, December 18 2018**

## **P2: Continuous degradation of toxic molecules through in-situ reduction of CO<sub>2</sub> using metal doped B-TiO<sub>2</sub> photocatalysts**

Hee Min Hwang<sup>1,2</sup>, Simgeon Oh<sup>1,2</sup>, Jinjoo Lee<sup>3</sup>, Yesel Hong<sup>3</sup>, G. Hwan Park<sup>3</sup>, Chang-il Shin<sup>3</sup>, Yerin Park<sup>3</sup>, Hyoyoung Lee<sup>1,2,3,\*</sup>

<sup>1</sup>Center for Integrated Nanostructure Physics (CINAP), Institute of Basic Science (IBS): 2066 Seoburo, Jangan-Gu, Suwon, Gyeonggi-Do 16419, Republic of Korea

<sup>2</sup>Department of Energy Science, Sungkyunkwan University: 2066 Seoburo, Jangan-Gu, Suwon, Gyeonggi-Do 16419, Republic of Korea

<sup>3</sup>Department of Chemistry, Sungkyunkwan University: 2066 Seoburo, Jangan-Gu, Suwon, Gyeonggi-Do 16419, Republic of Korea

\*Corresponding author. Email: hyoyoung@skku.edu

### **Abstract**

Up to now, complete water splitting reaction under sunlight for the continuous photo catalytic processes will be one of the most attractive methods to solve the future energy problems in the world. However, the problem of this reaction for the complete water splitting reaction requires sacrificial agents for hole scavenger such as methanol at the valence band (VB) and for electron scavenger such as AgNO<sub>3</sub> at the conduction band (CB) [1]. For the complete degradation of organic molecules using photocatalytic semiconducting materials such as TiO<sub>2</sub> [2], both activities at the valence band and conduction band sites are quite necessary for the continuous degradation process without using any scavengers.

In this report, we provide new continuous photo-catalytic processes through in-situ degradation of organic compounds at CB site and simultaneously conversion of CO<sub>2</sub> at VB site. B-TiO<sub>2</sub> was disordered rutile/ordered anatase TiO<sub>2</sub> phase-mixed structure via lithium-ethylenediamine (Li-EDA) treatment. The methyl paraoxon (MPO) is one of sarin simulants which are organophosphorus materials and toxic to human body. Degradation of MPO occurred on VB of B-TiO<sub>2</sub> to CO<sub>2</sub> and the resulting CO<sub>2</sub> was gradually converted to CO on CB of B-TiO<sub>2</sub>. We achieved 100 % degradation of nerve agent at CB and 72.09 % of conversion from CO<sub>2</sub> to CO (922.86 μmol/g) at VB of TiO<sub>2</sub>. It is first time to report for CO<sub>2</sub> reduction from nerve agents by using TiO<sub>2</sub>-based materials. As a whole, our concept can be applied for various environmental, military and energy conversion fields.

### **Keywords**

TiO<sub>2</sub>; degradation; CO<sub>2</sub> reduction; nerve agent; photocatalyst

### **References**

[1] S. R. Lingampalli, and C. N. R. Rao. Recent Progress in the Photocatalytic Reduction of Carbon Dioxide. ACS Omega. 2017, 2, 2740–2748

[2] Lizandra M. Zimmermann, Faruk Nome, Degradation of Methyl Paraoxon in the Presence of Mg<sup>2+</sup>-Al<sup>3+</sup> Mixed Oxides. J. Phys. Chem. C 2013, 117, 49, 26097-2610



**Poster Session**

**Room C, December 18 2018**

**P3: Ultraviolet photodetector using pn junction of p-CuO hollow nanospheres and n-ZnO nanorods**

Yuexing Ji<sup>1</sup>, Uijin Jung<sup>1</sup>, Jiyeon Yu<sup>1</sup>, Zhanpeng Xian<sup>1</sup>, Jinsub Park<sup>1,2,\*</sup>

<sup>1</sup>Department of Electronics and Computer Engineering, Hanyang University, Seoul 04763, Republic of Korea

<sup>2</sup>Department of Electronic Engineering, Hanyang University, Seoul 04763, Republic of Korea

\*Corresponding Author. Email: jinsubpark@hanyang.ac.kr

**Abstract**

Zinc oxide (ZnO) is a most well-studied n-type semiconductor for application of ultraviolet (UV) photodetectors due to its direct and wide energy band gap (~3.37 eV at room temperature). [1] But, UV photodetectors using ZnO show the low rising and falling time compare to other metal oxide materials. In order to improve these performances, we suggest new pn junction structure using p-CuO and n-ZnO for UV detector. At first we synthesize the p-CuO nanospheres by using polymer spheres template methods. The synthesized Cu-ion incorporated polymer spheres loaded on the top of n-ZnO nanorods (NRs) grown on n-Si substrate by hydrothermal method. The thermal annealing process changed monolayer of Cu-ion incorporated polymer spheres into CuO hollow nanospheres. In addition, the shrinkage of diameters of CuO occurred during the thermal annealing process resulting in formation of spacing between each sphere. To compare the effects of coverage of CuO nanospheres on device performance, we added another layer of CuO nanospheres with same process. The current-voltage (I-V) and time-related photocurrent (T-I) curves show that the fabrication of CuO nanospheres on ZnO could improve the detector performances. In addition, the sensitivity of 2-times transferred of CuO on the surface of n-ZnO NRs shows about 3 times higher than that of 1-time transferred CuO layer based detector. Our suggested p-CuO nanospheres covered n-ZnO NRs can improve the performance of UV photodetector which show the faster electron-hole separation and the suppression of recombination by the mutual transfer of the photo-generated electrons or holes. [2]

**Keywords**

CuO hollow nanospheres; pn junction; UV photodetector; Photo sensitivity

**References**

- [1] Anderson Janotti, Chris G Van de Walle, Fundamentals of zinc oxide as a semiconductor. Rep. Prog. Phys., 72, 126501 (2009)
- [2] Sheng-Bo Wang, Chih-Hung Hsiao, Shoou-Jinn Chang, Senior Member, IEEE, Z. Y. Jiao, Sheng-Joue Young, Shang-Chao Hung, and Bohr-Ran Huang, ZnO branched nanowires and the p-CuO/n-ZnO heterojunction nanostructured photodetector. IEEE Trans. Nanotechnol., 12, 263 (2013)

**Poster Session**

**Room C, December 18 2018**

**P4: Highly carbon-doped TiO<sub>2</sub> derived from MXene boosting the photocatalytic hydrogen evolution**

Guangri Jia, Ying Wang, Xiaoqiang Cui\*, Weitao Zheng\*

*Key Laboratory of Automobile Materials of MOE, School of Materials Science and Engineering, Jilin University, 2699 QianjinStreet, Changchun 130012, China*

\*Corresponding author. Email: xqcui@jlu.edu.cn, wtzheng@jlu.edu.cn (Weitao Zheng)

**Abstract**

The effective in situ carbon doping of titanium dioxide can greatly improve the lifetime of photogenerated carriers and widen the optical absorption range for photocatalytic reactions. [1] Here, highly carbon-doped TiO<sub>2</sub> (HC-TiO<sub>2</sub>) with a hierarchical structure and good crystallization was synthesized by using the exfoliated MXene at low temperature. [2] It was found that the high-content carbon doping induced a valence band tail state that promoted photogenerated carriers' effective separation and reduced bandgap, which greatly improved the utilization of light for photocatalytic reactions. This band tail was attributed to the strong electron withdrawing carboxylate groups from carbon doping. [3-4] The photocatalytic hydrogen production rate of the hierarchical HC-TiO<sub>2</sub> was 9.7 times that of the commercial P25 without cocatalyst under simulated sunlight. This work enriched the synthesis method of C-doped TiO<sub>2</sub> and the application of MXene based materials.

**Keywords**

Photocatalyst; Hydrogen evolution; C-TiO<sub>2</sub>; MXene; Hierarchical structure

**References**

- [1] Tian, J.; Zhao, Z.; Kumar, A.; Boughton, R. I.; Liu, H. Recent progress in design, synthesis, and applications of one-dimensional TiO<sub>2</sub> nanostructured surface heterostructures: a review. doi: 10.1039/C4CS00180J
- [2] Jia, G.; Wang, Y.; Cui, X.; Zheng, W., Highly carbon-doped TiO<sub>2</sub> derived from MXene boosting the photocatalytic hydrogen evolution. doi:10.1021/acssuschemeng.8b03406
- [3] Niu, P.; Wu, T.; Wen, L.; Tan, J.; Yang, Y.; Zheng, S.; Liang, Y.; Li, F.; Irvine, J. T. S.; Liu, G.; Ma, X.; Cheng, H. M. Substitutional carbon-modified anatase TiO<sub>2</sub> decahedral plates directly derived from titanium oxalate crystals via topotactic transition. doi: 10.1002/adma.201705999
- [4] Tao, J.; Luttrell, T.; Batzill, M. A two-dimensional phase of TiO<sub>2</sub> with a reduced bandgap. doi: 10.1038/nchem.1006

**Poster Session**

**Room C, December 18 2018**

## **P5: Hexagonal FeIn<sub>2</sub>S<sub>4</sub>: Layer Dependent Band Structure of Ternary Metal Chalcogenides**

Hyunjung Kim<sup>1,2</sup>, Hyoyoung Lee<sup>1,2,3,4,\*</sup>

<sup>1</sup>Centre for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS): Seobu-ro 2066, Suwon, Gyeonggi-do, Republic of Korea

<sup>2</sup>Sungkyunkwan University Advanced Institute of Nano Technology: Seobu-ro 2066, Suwon, Gyeonggi-do, Republic of Korea

<sup>3</sup>Department of Chemistry, Sungkyunkwan University (SKKU): Seobu-ro 2066, Suwon, Gyeonggi-do, Republic of Korea

<sup>4</sup>Department of Energy Science, Sungkyunkwan University (SKKU): Seobu-ro 2066, Suwon, Gyeonggi-do, Republic of Korea

\*Corresponding author. Email: hyoyoung@skku.edu

### **Abstract**

From the development of graphene, two dimensional nanomaterials have been widely studied due to their exotic characteristics. Among the several 2-dimensional materials such as graphene derivatives, hexagonal boron nitride, and phosphene, transition metal chalcogenides (TMDs) have received considerable attention due to their electrical characteristics, chemical stability and suitable band gaps for applications. [1] However, still there are only few studies for layered structure of ternary metal chalcogenides, which consists of two metal cations and one chalcogenide anions. Here, the layer dependence band gap the possibility of layer dependence of ternary metal chalcogenides was suggested with the hexagonal FeIn<sub>2</sub>S<sub>4</sub> (h-FIS) which was generally known as a spinel structure. [2] The investigation of formation of h-FIS was followed by comparison with cubic phase FeIn<sub>2</sub>S<sub>4</sub> (c-FIS) and hexagonal ZnIn<sub>2</sub>S<sub>4</sub>. The thickness of h-FIS was obtained by controlling the dissociation rate of sulfur radicals from sulfur precursor, [3] and then different band structure of each of h-FIS samples were investigated through the optical bandgap and redox potentials from cyclovoltammetry. This research will contribute to developing new applications of ternary metal chalcogenides and exploring their unveiled characteristics.

### **Keywords**

layered structure; iron indium sulfides; metal chalcogenides; two dimensional materials

### **References**

- [1] Butler SZ, Hollen SM, Cao L, Cui Y, Gupta JA, Gutiérrez HR, Heinz TF, Hong SS, Huang J, Ismach AF, Johnston-Halperin E, Kuno M, Plashnitsa VV, Robinson RD, Ruoff RS, Salahuddin S, Shan J, Shi L, Spencer MG, Terrones M, Windl W, Goldberger JE; Progress, challenges, and opportunities in two-dimensional materials beyond graphene. ACS Nano. 7(4), 2898 (2013). doi:10.1021/nn400280c
- [2] Kim H, Tiwari AP, Hwang E, Cho Y, Hwang H, Bak S, Hong Y, Lee H. FeIn<sub>2</sub>S<sub>4</sub> nanocrystals: A ternary metal chalcogenide material for ambipolar field-effect transistors. 5(7), 1800068 (2018). doi:10.1002/advs.201800068
- [3] Yoo D, Kim M, Jeong S, Han J, Cheon J. Chemical synthetic strategy for single-layer transition-metal chalcogenides. Journal of the American Chemical Society. 136(42), 14670-14673 (2014). doi:10.1021/ja5079943

**Poster Session**

**Room C, December 18 2018**

**P6: Ligand-exchanged colloidal WSe<sub>2</sub> and its counter cation dependent HER study**

Meeree Kim<sup>1,2</sup>, G. Hwan Park<sup>2</sup>, Yunhee Cho<sup>1,2</sup>, Yeseul Hong<sup>2</sup>, Hyoyoung Lee<sup>1,2,3,4,\*</sup>

<sup>1</sup>Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Sungkyunkwan University, Suwon, 16419, Republic of Korea

<sup>2</sup>Department of Chemistry, <sup>3</sup>Department of Energy Science and <sup>4</sup>Department of SAINT, Sungkyunkwan University (SKKU), Suwon, 16419, Republic of Korea

\*Corresponding author. Email: hyoyoung@skku.edu

**Abstract**

Hydrogen evolution reaction (HER) which involves the electrolysis of water molecules has been emerged as a clean synthesis of hydrogen, which is an alternative to steam methane reformer widely used in industry [1]. Promising candidates among earth-abundant catalysts are transition-metal dichalcogenides (TMDs), which are two-dimensional (2D) layered materials. They can reach high current densities at low over-potentials [2]. Commonly, these materials have been synthesized by vacuum-involving method like chemical vacuum deposition (CVD), while a colloidal synthesis has been less focused in spite of its scalable, less energy-intensive and cost-effective advantages [3]. The main reason is the presence of the surface ligands on the materials, resulting in the intrinsic limitation for use as catalysts.

In this study, we demonstrate the effectiveness of ligand-exchanged colloidal WSe<sub>2</sub> as a catalyst for HER. Up to now, it has been reported that the surface ligands can inhibit the catalytic reactions on the surface [3]; on the other hand, some other ligands have shown the lack of the inhibition effects [4] or even an increase in the reactivity [5]. As a layered material, WSe<sub>2</sub> has a potential to intercalate small molecules between its layers, and we found that after ligand exchange, this results in incorporation of charge-balancing counter cations into its layers which increases the current density. In this presentation, we like to introduce the study on HER activity by electrochemical measurement, XRD and XPS etc.

**Keywords**

Hydrogen evolution reaction (HER); Transition metal dichalcogenides (TMDs); Colloidal synthesis; Ligand exchange; Intercalation

**References**

- [1] N. Udengaard, Hydrogen Production by Steam Reforming of Hydrocarbons. Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem. 2004, 49, 906–907.
- [2] C. G. Morales-Guio; L.-A. Stern; X. Hu, Nanostructured Hydrotreating Catalysts for Electrochemical Hydrogen Evolution. Chem. Soc. Rev. 43, 6555 (2014). doi: 10.1039/C3CS60468C
- [3] D. A. Henckel; O. Lenz; B. M. Cossairt, Effect of Ligand Coverage on Hydrogen Evolution Catalyzed by Colloidal WSe<sub>2</sub>. ACS Catal. 7, 2815 (2017). doi: 10.1021/acscatal.7b00074
- [4] H. Borchert; D. Fenske; J. Kolny-Olesiak; J. Parisi; K. Al-Shamery; M. Baumer, Ligand-Capped Pt Nanocrystals as Oxide-Supported Catalysts: FTIR Spectroscopic Investigations of the Adsorption and Oxidation of CO. Angew. Chem., Int. Ed. 46, 2923 (2007). doi:10.1002/anie.200604460
- [5] Enhanced electrocatalysis of the oxygen reduction reaction based on patterning of platinum surfaces with cyanide. Nat. Chem. 2, 880 (2010). doi: 10.1038/nchem.771

**Poster Session**

**Room C, December 18 2018**

**P7: The Fabrication of ZnO Nanoarrays and Its Applications for Photoelectrochemical Water Splitting and Protein Microarray based Biosensing**

Chang Liu<sup>1</sup>, Lei Zhang<sup>1,2</sup>, Xiaoqiang Cui<sup>1,\*</sup>

<sup>1</sup>College of Materials Science and Engineering, Jilin University: No.2699 Qianjin Street, Changchun, China

<sup>2</sup>College of Chemistry, Jilin University: No.2699 Qianjin Street, Changchun, China

\*Corresponding author. Email: xqcui@jlu.edu.cn

**Abstract**

Nanostructured ZnO materials have received broad attention due to their distinguished performance in electronics, optics and photonics [1]. In this work, we designed and fabricated two ZnO nanoarrays composites including: CuO/ZnO nanoarrays heterojunction and ZnO NRs/Au film substrate. Here, we simultaneously improved the carrier separation and light harvesting by constructing P-N heterojunctions in CuO/ZnO nanoarrays composites. The CuO/ZnO nanoarrays heterojunction photoanode exhibited a significant negative shift of 150 mV for the onset potential and an approximately 4-fold enhancement in the photocurrent at 1.23 V vs RHE compared with those of pristine ZnO NRs. This work offers a facile strategy for preparing oxide-based P-N heterojunction photoanodes for enhanced PEC water splitting [2]. Moreover, we present the fabrication of a kind of novel plasmonic protein microarrays using nanostructured ZnO nanorod arrays (ZnO NRs) on 50 nm Au film that exhibits an enhancement of fluorescence up to 200-fold. The as-prepared plasmonic protein microarrays were used for the detection of the carcinoembryonic antigen (Carcinoembryonic Antigen, CEA) cancer biomarker. The plasmonic enhancement resulted in a detection limit of 27 pg mL<sup>-1</sup> in 0.01 M PBS and a dynamic range of 100 pg mL<sup>-1</sup> to 100 µg mL<sup>-1</sup>. The ZnO NRs/Au substrates can be mass-manufactured, which is highly promising for the development of low cost, sensitive, and high-throughput protein assay platform for applications in clinical diagnosis [3, 4]. These two ZnO nanoarrays composites would be further used in the field of PEC water splitting and protein microarray based biosensing.

**Keywords**

Zinc Oxide Nanoarrays (ZnO NRs); Photoelectrochemical Water Splitting; Heterojunction; Protein Microarray; Biosensing

**References**

- [1] W. Zhong Lin, Zinc oxide nanostructures: growth, properties and applications. *Journal of Physics: Condensed Matter*. 16, R829 (2004). doi:10.1088/0953-8984/16/25/R01
- [2] M. G. Walter; E. L. Warren; J. R. McKone; S. W. Boettcher; Q. Mi; E. A. Santori; N. S. Lewis, Solar Water Splitting Cells. *Chemical Reviews*. 110, 6446 (2010). doi:10.1021/cr1002326. doi:10.1002/adhm.201600414
- [3] C. Liu; F. Meng; B. Wang; L. Zhang; X. Cui, Plasmonic Nanograting Enhanced Fluorescence for Protein Microarray Analysis of Carcinoembryonic Antigen (CEA). *Analytical Methods*. 10, 145 (2018). doi:10.1039/C7AY02232H
- [4] C. Liu; F. Meng; W. Zheng; T. Xue; Z. Jin; Z. Wang; X. Cui, Plasmonic ZnO Nanorods/Au Substrates for Protein Microarrays with High Sensitivity and Broad Dynamic Range. *Sensors and Actuators B: Chemical*. 228, 231 (2016). doi:10.1016/j.snb.2016.01.019

**Poster Session**

**Room C, December 18 2018**

**P8: Electrochemical fabrication of hierarchical pseudocapacitive electrode for supercapacitor**

Yu Song, Xiaoxia Liu\*

*Chemistry Department, Northeastern University, Shenyang 110819, China*

\* Corresponding author. Email: xxliu@mail.neu.edu.cn

**Abstract**

Graphene has been received great attention as electrode materials for supercapacitor due to its high electrical conductivity, large surface area and perfect porosity effects. However, low capacitance of carbon-based materials limits their applications. In addition, pristine graphene is easy to restack. Incorporation of pseudocapacitive materials with graphene sheets is a good way to fabricate high performance supercapacitor electrode materials. However, in the composites made by in situ deposition of conducting polymers or inorganic oxides in suspensions of graphene sheets, connections between graphene sheets might be blocked by aggregations of the pseudocapacitive materials, so its effect on improving electric conductivity for the composites may be weakened.

A facile electrochemical method was designed by our group to prepare functionalized exfoliated graphite (FEG) with functionalized graphene sheets anchoring on the graphite substrates via a two-step partial exfoliation [1]. Nanostructured pseudocapacitive materials, such as MnO<sub>2</sub> and Ni-Co double hydroxide (Ni-Co DH), were electrochemically in situ grown on surfaces of graphene sheets in FEG to fabricate hierarchical pseudocapacitive electrodes [1-2].

**Keywords**

functionalized exfoliated graphite; MnO<sub>2</sub>; Ni-Co double hydroxide; supercapacitor

**Acknowledgments**

We gratefully acknowledge financial supports from National Natural Science Foundation of China (project number: 21673035).

**References**

- [1] Y. Song, D.-Y. Feng, T.-Y. Liu, Y. Li, X.-X. Liu, *Nanoscale*, 2015, 7, 3581–3587
- [2] Y. Song, X. Cai, X.-X. Xu, X.-X. Liu, *J. Mater. Chem. A*, 2015, 3, 14712-14720

**Poster Session**

**Room C, December 18 2018**

## **P9: Energy Band Modulation of Phase-selectively Disordered Pt-TiO<sub>2</sub> for Highly Active Photocatalysts**

Simgeon Oh<sup>1,3</sup>, Hee Min Hwang<sup>1,3</sup>, Doyoung Kim<sup>1,3</sup>, Joosung Kim<sup>1,3</sup>, GHwan Park<sup>1,2</sup>, Hyoyoung Lee<sup>1,2,3,\*</sup>

<sup>1</sup>Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Sungkyunkwan University, Suwon, 16419, Republic of Korea

<sup>2</sup>Department of Chemistry and <sup>3</sup>Department of Energy Science, Sungkyunkwan University (SKKU), Suwon, 16419, Republic of Korea

\*Corresponding author. Email: hyoyoung@skku.edu

### **Abstract**

P25 is a famous phase mixed TiO<sub>2</sub> with well lattice connected interface between anatase and rutile phase. This phase junction structure separates photo-exciton smoothly and its high photocatalytic performance reported by a number of papers.[1] And the continuous studies of P25 TiO<sub>2</sub> discovered that the outstanding charge separation performance of P25 occurred by low-energy electron transfer in type-I heterojunction energy band configuration between anatase and rutile phase TiO<sub>2</sub>. [2] In this study, we reduced Pt co-catalyst consumption for photocatalytic hydrogen evolution reaction (P-HER) by phase selective energy band modulation in P25 which has anatase and rutile two-phase mixed TiO<sub>2</sub> through our TiO<sub>2</sub> phase-selectively reduction method. An ordered anatase / disordered rutile and the disordered anatase / ordered rutile phase mixed P25 (OA/DR P25 TiO<sub>2</sub> and DA/OR P25 TiO<sub>2</sub>) synthesized and the type-II heterojunction energy band configuration achieved with OA/DR P25 TiO<sub>2</sub>. As a result, P-HER performance of OA/DR and DA/OR P25 TiO<sub>2</sub> samples showed improved performance and OA/DR P25 TiO<sub>2</sub> showed best performance than other TiO<sub>2</sub> samples due to it has only type-II heterojunction energy band configuration. Especially, P-HER performance test of OA/DR P25 TiO<sub>2</sub> with Pt deposition showed impressive P-HER performance with extremely low amount of Pt metal support. The Pt deposited OA/DR P25 TiO<sub>2</sub> (Pt-OA/DR P25 TiO<sub>2</sub>) performed higher hydrogen evolution rate with below 0.05 wt% Pt co-catalyst than Pt deposited P25 (Pt-P25) under simulated 1 sun irradiation whereas pristine P25 performed comparable hydrogen evolution rate with 0.5 wt% Pt co-catalyst. Consequently, Pt consumption of Pt-OA/DR P25 TiO<sub>2</sub> was 10 times lower than the Pt-P25 with energy band alignment. From the various band alignment measurements, we expected that the improper type-I heterojunction energy band alignment between anatase and rutile phase in pristine P25 hindered charge separation and carrier transfer process. [3] Whereas, the energy band modulated OA/DR P25 TiO<sub>2</sub> which has type-II heterojunction structure between anatase and rutile phase effectively separated photo-excited carriers and improved P-HER performance.

### **Keywords**

Photocatalyst; TiO<sub>2</sub>; Energy band modulation; Hydrogen evolution reaction

### **References**

- [1] B. Ohtani, O. O. Prieto-Mahaney, D. Li, R. Abe, What is Degussa (Evonik) P25? Crystalline composition analysis, reconstruction from isolated pure particles and photocatalytic activity test. *J Photochem Photobiol A Chem*, 216, 179 (2010). doi: 10.1016/j.jphotochem.2010.07.024
- [2] D. C. Hurum, A. G. Agrios, K. A. Gray, Explaining the Enhanced Photocatalytic Activity of Degussa P25 Mixed-Phase TiO<sub>2</sub> Using EPR. *J. Phys. Chem. B*, 107, 4545 (2003). doi: 10.1021/jp0273934
- [3] A. D. Paola, M. Bellardita, L. Palmisano, Brookite, the Least Known TiO<sub>2</sub> Photocatalyst. *Catalysts.*, 3, 36 (2013). doi:10.3390/catal3010036

**Poster Session**

**Room C, December 18 2018**

**P10: The effects of Ga<sub>2</sub>O<sub>3</sub> interlayer on the emission of n-In<sub>2</sub>O<sub>3</sub> nanorod/p-GaN heterojunction light emitting diode**

Dong Su Shin<sup>1</sup>, Dohyun Kim<sup>1</sup>, Subin Kim<sup>1</sup>, Jinsub Park<sup>1,2,\*</sup>

<sup>1</sup>Department of Electronics and Computer Engineering, Hanyang University, Seoul 04763, Republic of Korea

<sup>2</sup>Department of Electronics Engineering, Hanyang University, Seoul 04763, Republic of Korea

\*Corresponding author. Email: jinsubpark@hanyang.ac.kr

**Abstract**

The In<sub>2</sub>O<sub>3</sub> has been used for various opto-electrical devices such as photodetector, gas sensor, transistor, and transparent conducting electrode [1] due to its large band gap (3.4 eV at room temp) and high mobility (160 cm<sup>2</sup>/V·s). Despite of its optical and structural merits, light emitting diode using In<sub>2</sub>O<sub>3</sub> nanostructure has not yet been reported [2]. In this study, we report on the effects of formation of Ga<sub>2</sub>O<sub>3</sub> on p-GaN surface by O<sub>2</sub> plasma treatment on morphological property of post-grown In<sub>2</sub>O<sub>3</sub> nanorods(NRs) to fabricate n-In<sub>2</sub>O<sub>3</sub>/p-GaN pn heterojunction based light emitting diode. After formation of Ga<sub>2</sub>O<sub>3</sub> layer on p-GaN surface, the transformation of surface property from hydrophobic to hydrophilic property makes possible to grow of uniformed In(OH)<sub>3</sub> NRs on p-GaN surface by using hydrothermal method [3]. Through the calcination process conducted at 600 °C in air ambient, In(OH)<sub>3</sub> NRs were changed to In<sub>2</sub>O<sub>3</sub> NRs without the severe morphology changes. After fabrication of LED devices using the general photolithography and electrode deposition method, the current-voltage (I-V) measurements are conducted. The obtained I-V curve of n-In<sub>2</sub>O<sub>3</sub> NRs/p-GaN with Ga<sub>2</sub>O<sub>3</sub> interlayer shows rectified diode characteristics and turn-on voltage of 12.6 V at forward bias condition with green light emission ( $\lambda \sim 554$  nm). As a possible green light emission mechanism from our suggested structures, the various defects energy states mediated green emissions were considered.

**Keywords**

Surface treatment; Green emission; Ga<sub>2</sub>O<sub>3</sub>; In<sub>2</sub>O<sub>3</sub> nanorods

**References**

- [1] J.H.W. De Wit, G. Van Unen, M. Lahey, Electron concentration and mobility in In<sub>2</sub>O<sub>3</sub>. J. Phys. Chem. Solids 38, 819 (1977). doi: 10.1016/0022-3697(77)90117-2
- [2] D. Shao, L. Qin, S. Sawyer, High Responsivity, Bandpass Near-UV Photodetector Fabricated From PVA-In<sub>2</sub>O<sub>3</sub> Nanoparticles on a GaN Substrate, IEEE Photon. J. 4, 715(2012). doi:10.1109/JPHOT.2012.2195485
- [3] R. Su, H. Liu, T. Kong, Q. Song, N. Li, G. Jin, G. Cheng, Tuning Surface Wettability of In<sub>x</sub>Ga<sub>(1-x)</sub>N Nanotip Arrays by Phosphonic Acid Modification and Photoillumination, Langmuir 27, 13220(2011). doi:10.1021/la203072n



**Poster Session**

**Room C, December 18 2018**

**P11: Impacts of Zr-doping into crystalline lattices of bismuth vanadate powder and thin film on their photocatalytic and photoelectrochemical properties**

Takato Kawaguchi<sup>1</sup>, Yui Higuchi<sup>1</sup>, Naoto Kawasaki<sup>1</sup>, Takashi Harada<sup>2</sup>, Mikas Remeika<sup>3</sup>, Muhammad Monirul Islam<sup>3</sup>, Takeaki Sakurai<sup>3</sup>, Shigeru Ikeda<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science and Engineering Konan University, 8-9-1 Okamoto, Higashinada, Kobe 658-8501, Japan

<sup>2</sup>Research Center for Solar Energy Chemistry, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan

<sup>3</sup>Institute of Applied Physics, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan

\*Corresponding author: +81-78-435-2494, s-ikeda@konan-u.ac.jp

**Abstract**

Bismuth vanadate (BiVO<sub>4</sub>) has been studied extensively as a potential photocatalyst and/or photoanode for oxygen (O<sub>2</sub>) production through water-splitting using sunlight [1]. BiVO<sub>4</sub> possess two doping sites, Bi and V. So far, doping with molybdenum (Mo) or tungsten (W) at the V site has shown to be effective to enhance activity for water oxidation [2]. Since hexavalent form is the most stable phase for Mo and W, doping with these elements at the pentavalent V site should introduce excess electrons. Hence increasing in n-type conductivity would be effective for the enhancement of the activity. In accordance with the study of density functional theory (DFT) reported by Yin et al., group IVB elements such as Zr and Hf can substitute the Bi site in BiVO<sub>4</sub> because of its low formation energy [3]. Since replacements of trivalent Bi with tetravalent Zr and Hf should induce increments of n-type conductivity, these electrostructural changes would be beneficial for the improvement of photocatalytic water oxidation. In the present study, therefore, effects of zirconium (Zr) doping into the BiVO<sub>4</sub> powder on its structural and photocatalytic activity for O<sub>2</sub> evolution were examined. The formation of the BiVO<sub>4</sub> powder crystallized in the monoclinic scheelite structure (*ms*-BiVO<sub>4</sub>) was achieved when the sample doped with relatively small amount of Zr. The photocatalytic activity of the Zr-doped *ms*-BiVO<sub>4</sub> powder showed much higher than that of non-doped *ms*-BiVO<sub>4</sub>. However, further doping induced structural alterations into tetragonal scheelite and tetragonal zircon structures, leading to lowering photocatalytic activity for O<sub>2</sub> evolution. Similar effects of Zr doping were also confirmed by the photoelectrochemical (PEC) system based on the BiVO<sub>4</sub> thin film doped with various amounts of Zr. Thus, the Zr doping was confirmed to be effective for improvements of photocatalytic/(PEC) functions of BiVO<sub>4</sub> for water oxidation.

**Keywords**

Zr-doping, photocatalytic water oxidation, crystalline structure.

**References**

- [1] A. Kudo, K. Omori, H. Kato, J. Am. Chem. Soc. 121 (1999) 11459.
- [2] H. S. Park, K. E. Kweon, H. Ye, E. Paek, G. S. Hwang, A. J. Bard, J. Phys. Chem. C, 115 (2011)
- [3] W.-J. Yin, S.-H. Wei, M. M. Al-Jassim, J. Turner, Y. Yan, Phys. Rev. B 83 (2011) 15510

**Poster Session**

**Room C, December 18 2018**

**P12: Silver-incorporated Cu<sub>2</sub>ZnSnS<sub>4</sub> thin film as an absorber for solar cells and a cathode for photoelectrochemical water splitting**

Takato Kawaguchi<sup>1</sup>, Thi Hiep Nguyen<sup>2</sup>, Takashi Harada<sup>2</sup>, Shuji Nakanishi<sup>2</sup>, Masanobu Higashi<sup>3</sup>, Ryu Abe<sup>3</sup>, Shigeru Ikeda<sup>1,\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science and Engineering, Konan University, 8-9-1 Okamoto, Higashinada, Kobe 658-8501, Japan

<sup>2</sup>Research Center for Solar Energy Chemistry, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan

<sup>3</sup>Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto University, Katsura Nishikyo-ku, Kyoto 615-8510, Japan

\*Corresponding author. Email: s-ikeda@konan-u.ac.jp

**Abstract**

Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) is a promising absorber material for photovoltaic (PV) solar cells as well as a photocathode for photoelectrochemical (PEC) water splitting and carbon oxide fixation [1-4]. We have recently demonstrated successful fabrication of CZTS film with sufficient qualities for PV and PEC applications by using a facile spray pyrolysis method [5-7]. For further improvements of PV and PEC properties, impacts of silver (Ag) incorporation into the crystalline lattice of CZTS on its structural, optical, and electric properties were examined.

Crystallographic analyses indicated successful incorporation of various amounts of Ag up to an Ag / (Ag + Cu) ratio of ca. 0.1 into the crystal lattice of CZTS without formation of other impurity compounds. Appreciable enhancements of PV properties and PEC water splitting performances were obtained by the Ag incorporation. Electrostructural analyses of the devices suggested that the Ag-incorporated film in the device achieved reduction in the amounts of unfavorable copper on zinc antisite defects in comparison with those in the bare CZTS film. Moreover, the use of an Ag-incorporated film improved band alignment at the CdS(buffer)-CZTS interface.

**Keywords**

Cu<sub>2</sub>ZnSnS<sub>4</sub> thin films; Ag incorporation; defect concentrations

**References**

- [1] H. Katagiri, K. Jimbo, W. S. Maw, K. Oishi, M. Yamazaki, H. Araki, A. Takeuchi, *Thin Solid Films*, 517 (2009) 2455
- [2] F. Liu, C. Yan, J. Huang, K. Sun, F. Zhou, J. A. Stride, M. A. Green, X. Hao, *Adv. Energy Mater.*, 6 (2016) 1600706
- [3] S. Kamimura, Y. Sasaki, M. Kanaya, T. Tsubota, T. Ohno, *RSC Adv.*, 6 (2016) 112594
- [4] K. Iwashina, A. Iwase, Y. H. Ng, R. Amal, A. Kudo, *J. Am. Chem. Soc.*, 137 (2015) 604
- [5] T. H. Nguyen, W. Septina, S. Fujikawa, F. Jiang, T. Harada, S. Ikeda, *RSC Adv.*, 5 (2015) 77565
- [6] T. H. Nguyen, T. Harada, J. Chantana, T. Minemoto, S. Nakanishi, S. Ikeda, *ChemSusChem*, 9 (2016) 2414
- [7] T. H. Nguyen, T. Harada, S. Fujikawa, S. Nakanishi, S. Ikeda, *ECS Trans*, 75 (2017) 15

**Poster Session**

**Room C, December 18 2018**

**P13: Graphene quantum dots decorated graphene as an enhanced sensing platform for sensitive and selective detection of copper(II)**

Ying Wang, Guangri Jia, Xiaoqiang Cui\*

*Jilin University, 2699 Qianjin Street, Changchun, China*

\*Corresponding author. Email: xqcui@jlu.edu.cn

**Abstract**

It is essential to develop high sensitive and selective methods for monitoring and measuring of the trace Cu(II). [1-3] Based on this urgent demand, we designed a simple and efficient electrochemical sensing platform based on the hybrid of two carbon nanomaterials for the sensitive and selective detection of trace Cu(II) by using differential pulse anodic stripping voltammetry (DPASV) analysis. The GQDs/graphene/GCE exhibited enhanced electrochemical responses because of a fast electron transfer from graphene and a high affinity to Cu(II) from graphene quantum dots (GQDs). Under the optimal conditions, a good linear response in the range of 0.015 – 8.775  $\mu\text{M}$  with correlation coefficient of 0.9995 and a detection limit of 1.34 nM ( $S/N = 3$ ) were obtained. The developed method was further validated and successfully applied to the detection of Cu(II) in real water samples. The simple preparation and efficient selectivity of the proposed modified electrode show the promising potential for applications in sensing of Cu(II).

**Keywords**

Electrochemical sensor; Graphene; Graphene quantum dots; Copper(II)

**References**

- [1] A. Ambrosi, C.K. Chua, N.M. Latiff, A.H. Loo, C.H.A. Wong, A.Y.S. Eng, A. Bonanni, M. Pumera, Graphene and its electrochemistry—an update, *Chem. Soc. Rev.* 45, 2458 (2016). doi: 10.1039/c6cs00136j
- [2] Z. Zhang, J. Zhang, N. Chen, L. Qu, Graphene quantum dots: an emerging material for energy-related applications and beyond, *Energ. Environ. Sci.* 5, 8869 (2012). doi: 10.1039/c2ee22982j
- [3] Y. Wang, S. Zhao, J. Qi\*, X. Cui\*, Graphene quantum dots decorated graphene as an enhanced sensing platform for sensitive and selective detection of copper(II), *J. Electro. Chem.* 797, 113 (2017). doi: 10.1016/j.jelechem.2017.05.031

**Poster Session**

**Room C, December 18 2018**

**P14: Elastic nanoscale spongy graphene-functionalized silicon as excellent stability anode in Li ion battery**

Chunfei Zhang, Byong-June Lee, Jong-Sung Yu\*

*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu 42988, Republic of Korea*

\*Corresponding author. Email: jsyu@dgist.ac.kr

**Abstract**

Silicon can make alloy with lithium in the form of  $\text{Li}_{22}\text{Si}_5$  to deliver a highest theoretical gravimetric capacity of  $\sim 4200 \text{ mAh g}^{-1}$ , and thus is considered to be one of the most promising anode materials for next generation Li ion battery. However, those advantages are seriously offset by a great challenge of large volume expansion during lithiation, which causes a serious damage to the electrode structure and thus gives rise to a fast decay of the specific capacity [1]. In this work, novel 3D spongy graphene (SG)-functionalized silicon is for the first time demonstrated by chemical vapor deposition for a LIB anode, which can overcome the common silicon anode issues such as poor conductivity and volume expansion of Si as well as transfer of Li ion towards the Si. The elastic feature of graphene has excellent function to self-adaptively buffer the volume variation during charge-discharge process. In addition, different from traditional graphene or carbon shells (core-shell and yolk-shell), the spongy 3D graphene networks provide much improved unique functions with excellent long-cycle stability and rate capability. The Si@SG electrode exhibits excellent cycling performance with high reversible specific capacity [2]. A superior 95% capacity retention is achieved after 510 cycles.

**References**

- [1] M. Zhou, X. Li, B. Wang, Y. Zhang, et al. *Nano Lett.* 15 (2015) 6222-6228
- [2] C. Zhang, T.-H. Kang, J.-S. Yu, *Nano Research*, 11(2018) 233-245

**Poster Session**

**Room C, December 18 2018**

**P15: Structure and visible-light induced photocatalytic activity of metal cyanamide composites**

Hao Meng, Yu Wang, Xia Zhang\*

*Department of chemistry, Northeastern University. Wenhua Road/Box332, Shenyang, Liaoning, China*

\*Corresponding author. Email: xzhang@mail.neu.edu.cn

**Abstract**

Photocatalytic technology can utilize solar energy as induced light to degrade various organic pollutants and produce hydrogen from water splitting, which shows broad prospect applications in the development of new energy and environmental pollution treatment [1]. Metal cyanamide is a new type of photocatalysts. Theoretically, cyanamide ion ( $[\text{NCN}]^{2-}$ ) is a linear ion composed of three atoms, which can form metal-metal bridged compounds. And the delocalized  $\pi$  conjugation can be formed by atoms C and N through  $\text{SP}^2$  hybridization, which electronic structure in HOMO and LUMO orbitals is more similar with that of carbides or sulfides, and therefore exhibits good visible light response and photocatalytic activity [2]. In this study, some single metal cyanamide such as  $\text{ZnNCN}$ ,  $\text{Ag}_2\text{NCN}$ ,  $\text{Ni}(\text{HNCN})_2$  and  $\text{CdNCN}$  have been synthesized by a simple ligand exchange method. Their photo response, band structure and photocatalytic activity are studied respectively. These metal cyanamide were then hybridized with traditional inorganic conductors, such as  $\text{TiO}_2$  and  $\text{BiVO}_4$ , and the charge transfer at the interface of hetero structure and photocatalytic mechanism have been proposed too. Compared to the single metal cyanamide, the nanocomposites of  $\text{Ag}_2\text{NCN}/\text{TiO}_2$  [3],  $\text{Ag}_2\text{NCN}/\text{ZnNCN}$  and  $\text{Ni}(\text{HNCN})_2/\text{BiVO}_4$  all exhibit enhanced photocatalytic activity owing to the effective charge separation because of the matched energy bands of hetero components.

**Keywords**

Visible-light induced photocatalysis; Metal cyanamide; Nanocomposites; Interface control; Photocatalytic mechanism

**References**

- [1] A. Fujishima; K. Honda K, Electronchemical Photolysis of Water at Semiconductor Electrode. *Nature*. 238, 37 (1972). doi:10.1038/238037a0
- [2] W. Zhao; Y. Liu; J. Liu; P. Chen; I. W. Chen; F. Huang; J. Lin, Controllable Synthesis of Silver Cyanamide as a New Semiconductor Photocatalyst under Visible-light Irradiation. *Journal of Materials Chemistry*. 1, 7942 (2013). doi:10.1039/C3TA10868F
- [3] H. Meng; X. X. Li; X. Zhang; Y. F. Liu; Y. Xu; Y. D. Han; J. L. Xu, Fabrication of Nanocomposites Composed of Silver Cyanamide and Titania for Improved Photocatalytic Hydrogen Generation. *Dalton Transactions*. 44, 19948 (2015). doi: 10.1039/c5dt03869c

**Poster Session**

**Room C, December 18 2018**

## P16: Nanoporous Sulfur-doped Copper Oxide ( $\text{Cu}_2\text{O}_x\text{S}_{1-x}$ ) for Overall Water Splitting

Xiaolin Zhang, Xiaoqiang Cui\*, Yuanhui Sun, Kun Qi, Zhao Jin, Shuting Wei, Weiwei Li, Lijun Zhang, Weitao Zheng\*

*State Key Laboratory of Automotive Simulation and Control, Department of Materials Science and Key Laboratory of Automobile Materials of MOE, Jilin University, 2699 Qianjin Street, Changchun 130012, People's Republic of China*

\*Corresponding author. Email: xqcui@jlu.edu.cn (Xiaoqiang Cui), wtzheng@jlu.edu.cn (Weitao Zheng)

### Abstract

Developing active and bifunctional noble metal-free electrocatalysts is crucial for both the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in the full water splitting process. [1-3] A ternary nanoporous sulfur doped copper oxide ( $\text{Cu}_2\text{O}_x\text{S}_{1-x}$ ) was successfully synthesized on Cu foam. The obtained  $\text{Cu}_2\text{O}_x\text{S}_{1-x}/\text{Cu}$  shows robust electrocatalytic activity towards HER with a low overpotential of 40 mV at  $10 \text{ mA cm}^{-2}$ , a Tafel slope of  $68 \text{ mV dec}^{-1}$ , and exhibits long-term stability in acid solution. [4] Moreover, the  $\text{Cu}_2\text{O}_x\text{S}_{1-x}$  shows excellent electrocatalytic activity for OER, HER, and overall water splitting as a bifunctional catalyst in 1.0 M KOH electrolyte. The sulfur doping strategy implemented here can greatly improve the catalytic performance and stability in both acidic and alkaline water electrolyzers and presents an efficient catalyst for overall water splitting.

### Keywords

$\text{Cu}_2\text{O}_x\text{S}_{1-x}$ ; sulfur doping; hydrogen evolution reaction; oxygen evolution reaction; overall water splitting

### References

- [1] Wang, J.; Xu, F.; Jin, H.; Chen, Y.; Wang, Y., Non-Noble Metal-based Carbon Composites in Hydrogen Evolution Reaction: Fundamentals to Applications. *Advanced Materials* 2017, 29 (14), 1605838. doi: 10.1002/adma.201605838
- [2] Wang, J.; Cui, W.; Liu, Q.; Xing, Z.; Asiri, A. M.; Sun, X., Recent Progress in Cobalt-Based Heterogeneous Catalysts for Electrochemical Water Splitting. *Advanced Materials* 2016, 28 (2), 215-230. doi: 10.1002/adma.201502696
- [3] Du, P.; Eisenberg, R., Catalysts made of earth-abundant elements (Co, Ni, Fe) for water splitting: Recent progress and future challenges. *Energy & Environmental Science* 2012, 5 (3), 6012-6021. doi: 10.1039/c2ee03250c
- [4] Zhang, X.; Cui, X.; Sun, Y.; Qi, K.; Jin, Z.; Wei, S.; Li, W.; Zhang, L.; Zheng, W.; *ACS Applied Materials Interfaces*, 2018, 10, 745-752. doi:10.1021/acsami.7b16280

## Author Index

Ricky Lay-Kee Ang	11	Chang Liu	87
Abul K. Azad	41	Huan Liu	27
A.O. Antonenko	7	Jianguo Liu	26
Arun Bansil	1	Xiaoxia Liu	88
Rodolphe Antoine	74	Yo-Sep Min	17
Myung-Ho Bae	63	Oleg V. Misochko	39
S. Boonchui	56	Indrajit Mukhopadhyay	38
Ray T. Chen	46	Tomohiko NAKAJIMA	44
Ah-Jin Cho	20	Yoshitaro NOSE	43
Yunhee Cho	81	Simgeon Oh	89
Zhifei Dai	67	Jinsub Park	49
Ioana Demetrescu	65	Rosaria Puglisi	54
Emiliano Descrovi	47	Xinhua Qi	22
Yuan Dong	53	Shivendu Ranjan	80
S. F. Fischer	5	Sekhar Chandra Ray	8
Lu Gan	23	Jaime Gómez Rivas	28
Amanda F. Gouveia	21	Hiroshi Sakaguchi	36
Hongchen Gu	79	Liwen Sang	18
Raju Kumar Gupta	25	Sohyeon Seo	29
Jisang Hong	40	Feng Shen	59
Yan Hong	50	Makoto Shimizu	15
Lingling Huang	48	Dong Su Shin	90
Xianjun Huang	35	Raman Singh	2
Dae Kun Hwang	69	Amna Sirelkhatim	71
Hee Min Hwang	82	Bunned Soodchomshom	33
Shigeru Ikeda	42	Sukrit Sucharitakul	60
Seongil Im	62	Katsuhisa Taguchi	3
Su-il In	14	Palanisamy Thanikaivelan	76
Yuexing Ji	83	Elijah Thimsen	24
Guangri Jia	84	Rohit Tripathi	34
Jiang Jiang	66	Yen Nee Tan	77
Sang-Yong Ju	12	Peng Wang	61
Mukul Kabir	55	Ying Wang	93
Hyunjung Kim	85	Yang Yan	57
Takato Kawaguchi	91,92	Taka-aki Yano	52
Meeree Kim	86	Long-Jing Yin	6
Young-Kuk Kim	19	Jiashing Yu	75
Young Jun Kim	70	Jong-Sung Yu	94
Oleg V. Kononenko	9	Xia Zhang	95
Hansang Kwon	10	Xiaolin Zhang	96
Hyoyoung Lee	13	Xu Zhang	37
Xiaowei Li	51	Xudong Zhao	45
Jarrn-Horng Lin	64	Yanzhong Zhang	73