



US-China Workshop 中美論壇



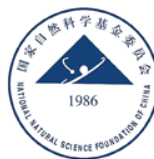
on Nanostructured Materials for Global Energy and Environmental Challenges



**Evanston, Illinois
September 22-24, 2008**



**National Science
Foundation**



**National Natural Science
Foundation of China
國家自然科學基金委員會**

Table of Contents

	Page
Acknowledgements	3
Section 1: Executive Summary	5
Section 2: Participants	6
Section 3: Program Highlights	7
Section 4: Group Recommendations	14
Section 5: Implementation Strategy	19
Section 6: Conclusions	20
<u>Appendices</u>	
Appendix 1: Participant List	21
Appendix 2: Program	24
Appendix 3: Abstracts for Talks and Posters	27
Appendix 4: Research Abstracts of Chinese Delegates	37
Appendix 5: Working Group Guidelines	44
Appendix 6: Group Reports	45

Acknowledgements

As co-organizers of the Workshop, we gratefully acknowledge the funding and visionary leadership of the National Science Foundation (NSF) and the National Natural Science Foundation of China (NSFC) and thank them for the honor of organizing this important event.

We would also like to thank

...the members of both agencies who took time to attend this Workshop and share information about US and Chinese funding mechanisms;

...the Chinese delegates for making the long trip from China and the US researchers and students who traveled from different parts of the country in the spirit of international cooperation. Their valuable contributions have made this first bilateral workshop a great success;

...the Northwestern University administration for their generous support of this Workshop, particularly Jay Walsh, Vice President for Research, Julio Ottino, Dean of the McCormick School for Engineering and Applied Mathematics, and Richard Leuptow, Senior Associate Dean for Operations and Research at the McCormick School;

...the staff of the Northwestern Materials Research Institute for their excellent organization and support, including Jennifer Shanahan, Chooi Lou, Jim Chen, Fei Yeh, Melinda Wong, Peng Liu, Meng Wei Liu, Megan O'Sullivan and John Brundage; and

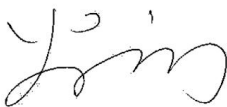
...the assistants of the Institute of Energy Materials and Ecomaterials in China for their excellent support, including Bing Wang, Rui Ran, Jun Fan and Jia Li.

We look forward to many more bilateral workshops in this series, beginning next year in China!

Workshop Co-organizers



R.P.H. Chang
Northwestern University



Duan Weng
Tsinghua University



Section 1: Executive Summary

The US and China both consume large amounts of energy and produce large amounts of environmental pollutants, resulting in climate change, health risks, and other global problems. In response to these shared challenges, the Natural National Science Foundation of China (NSFC) and the US National Science Foundation (NSF) have launched a series of co-sponsored bilateral workshops to foster US-China cooperation and establish new mechanisms to support collaborative research, education, and networking in these critical areas.

The first of this series – the US-China Workshop on Nanostructured Materials for Global Energy and Environmental Challenges - was held September 22-24, 2008 in Evanston, Illinois. Co-organized by R.P.H. Chang of Northwestern University (US) and Duan Weng of Tsinghua University (China), the workshop assembled experts from the US and China to discuss two major themes: (1) Advanced Solar Cells and (2) Nanomaterials and the Environment. In attendance were more than 60 invited researchers, students and observers from academia, industry, national labs, and government funding agencies in China and the US.

The workshop program was designed to accomplish the following goals.

1. Identify potential research areas/topics to address shared energy and environmental challenges facing the US and China.
2. Generate recommendations for addressing these challenges together, including potential jointly funded research projects between the US and China.
3. Establish active US-China working groups in these areas, as part of the Materials World Network.

Day 1 consisted of information sharing via talks, panel discussions, and a student poster session. On Days 2 and 3, participants broke into working groups to generate recommendations and potential projects.

The primary and overarching finding of this Workshop is that solving global energy and environmental challenges will require transformative approaches and new levels of cooperation. Among the key recommendations to emerge from the working group sessions was the establishment of a jointly funded and operated US-China institute that would provide a seamless, sustainable environment for long-term collaborative research, education and networking. By virtue of its joint ownership, extended lifespan, and broad scope, such an institute would eliminate many existing barriers to successful US-China collaborations and foster transformative research for rapidly solving urgent global energy and environmental challenges. This new paradigm is a major deliverable of the Workshop, and one that presents stakeholders in the US and China – industry, government agencies, universities, national laboratories, centers and institutes – with a significant challenge and call-to-action.

Participants also called for much to be done in the near term. They identified numerous areas for potential collaboration and expanded many of these into detailed projects for potential funding under the NSF Materials World Network framework and other existing programs. They recommended that database be created to exchange complementary expertise and resources in both countries and link potential collaborators on both sides. Their recommendations to improve networking included expanding student involvement, launching a university network, improving

cyberinfrastructure-based communication, and organizing more US-China workshops, some on narrow research foci and others to identify and address “grand challenges.” In the area of education, they recommended increased student exchange over longer periods, more opportunities for US students to visit and perform research in China, and specific improvements to existing NSF programs such as the Research Experience for Undergraduates (REU) and the Graduate Research Fellowships program.

The second workshop in this series, planned for China in 2009, will be an opportunity to implement many of these recommendations. In the meantime, the group reports will be a useful resource for the funding agencies in their ongoing efforts to support US-China cooperation. Participants are encouraged to continue using the workshop cyberinfrastructure (www.materialsworld.net) for ongoing discussions and implementation. The organizers will launch quarterly discussions to maintain momentum.

Section 2: Participants

More than 60 researchers, students and observers from the US and China attended the Workshop (see Appendix 1 for the participant list.)

Participation was by invitation only. Both sides worked conscientiously to assemble a diverse group of attendees from academia, industry and national laboratories representing different regions of the US and China, with an emphasis on diversity of gender, ethnicity, career level and discipline. Participants came from materials science, chemistry, mathematics, chemical engineering, electrical engineering, environmental engineering, policy and other fields.

The co-organizers worked with the NSF and the NSFC to ensure representation by leading solar cell researchers, nanomaterials experts, and environmental scientists and engineers. In attendance were twenty-three invited researchers from the US and nine invited researchers from China. The original Chinese delegation included almost twice as many invited researchers. Unfortunately, many encountered visa problems and were unable to attend.



Graduate student Giriprasath Gururajan of the University of Delaware presents his research

Student participation was emphasized. Participating researchers were asked to nominate their best graduate students and postdocs to accompany them to the Workshop. Financial support was provided to cover student travel and lodging. Ten graduate students and one postdoc attended the Workshop, where they listened to talks and panel presentations, presented research posters, and joined working group breakout sessions. They also shared rooms with young researchers from different institutions, which fostered informal networking among the students. It is hoped that future workshops in this series will involve larger numbers of students.



Assistant Professor, Thuc-Guyen Nguyen of UC Santa Barbara questions the panel.

Observers included ten government agency representatives from the US and China. The NSF was represented by three divisions within the Directorate for Mathematical and Physical Sciences – the Division of Materials Research (DMR), the Division of Chemistry (CHE), and the Division of Mathematical Sciences (DMS). The NSFC was represented by the Bureau of Engineering and Materials, the Division of Ceramics Materials (Bureau of Engineering and Materials), the Division of Metal Materials (Bureau of Engineering and Materials), and the Division of America and Atlantic (Bureau of International Cooperation). Agency representatives also met privately to discuss joint funding mechanisms and programs to foster US-China cooperation.



S. Marder of Georgia Tech, M. Wasielewski of Northwestern, Wei Qin of the NSFC, and Feiyu Kang of Tsinghua University

Participants were encouraged to begin interacting several months before the Workshop via a private community-based cyberinfrastructure consisting of searchable research profiles, group workspaces, document repositories, and discussion forums. These tools remain available to support ongoing discussions (www.materialsworld.net).

Section 3: Program Highlights

The program was designed to support the goals of the Workshop. Day 1 consisted of information exchange through speaker sessions, panel discussions and a student poster session. Day 2 began with an introduction of joint NSF and NSFC funding mechanisms, followed by working group discussions and reporting. NSF-NSFC representatives also met in a closed parallel session to discuss the development of joint funding mechanisms and programs to foster US-China cooperation. Day 3 consisted of group reporting. Program highlights are given below.

The full workshop program can be found in Appendix 2.

Opening Remarks

The co-organizers welcomed participants and outlined the goals of the Workshop. NSF and NSFC leaders described the origins and objectives of the bilateral Workshop series.



Zakya Kafafi, Director, Division for Materials Research, NSF



Louis Echegoyen, Director, Division of Chemistry, NSF



Ruiping Gao, Deputy Director, Bureau of Engineering and Materials, NSFC

Speaker Session 1: Nanomaterials and the Environment

- “State-of the-art of Ecomaterials in China,” Duan Weng, Professor of Nanomaterials and Environment at Tsinghua University (China)
- “Nanoparticles in the Environment: The Measurement Challenge,” Richard Flagan, Professor of Chemical Engineering and Professor of Environmental Science and Engineering at the California Institute of Technology (US)



Speaker Session 2: Advanced Solar Cells

- “Achieving High Performance Solar Cells through Innovative Approaches,” Yang Yang, Professor of Materials Science and Engineering at University of California at Los Angeles
- “Studies and Recent Progress of Polymer Bulk-Heterojunction Photovoltaic Devices,” Yong Cao, Institute of Polymer Optoelectronic materials and Devices, South China University of Technology, Guangzhou (China)

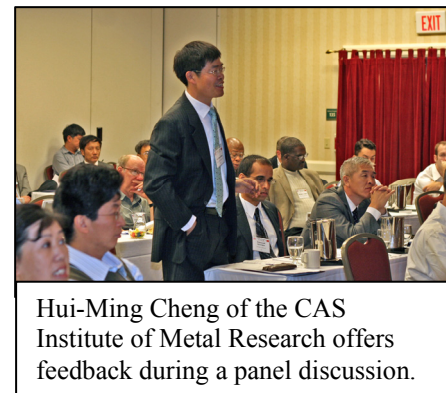
Panel 1: Nanomaterials Synthesis



- Hui-Ming Cheng, Professor of IMR at Institute of Metal Research, Chinese Academy of Sciences (China) with research interests in synthesis, characterization and applications of carbon nanotubes and other nanostructures, high-performance hydrogen storage materials, and materials and devices for efficient solar energy conversion.
- Jian Xu, Professor of IMR at the Institute of Chemistry, Chinese Academy of Sciences (China) with research interests in polymer physics including advanced materials of functional polymer and optical polymer fiber.
- Olivia Graeve, Professor of Materials Science and Engineering at Alfred University (US) with research interests in processing of transparent ceramics for optical applications, processing of carbide powders for high-temperature applications, and synthesis and characterization of functional ceramics.
- Stefan Bernhard, Professor of Chemistry at Princeton University (US) with research interests in synthesis of novel supramolecular systems, polymers and extended structures for materials applications.

Panel 2: Nano Characterization Techniques

- Zhanquo Wang is a Professor of IS at the Institute of Semiconductors, Chinese Academy of Sciences (China) with research interests in semiconductor nanostructures growth and related quantum devices fabrication.
- Yunqi Liu, Professor at the Institute of Chemistry, Chinese Academy of Sciences (China) with research interests in design and synthesis of molecular materials, organic/polymeric light-emitting diodes, organized field-effect transistors, and preparation of carbon nanotubes and electronic devices.
- Bruce Parkinson is a Professor of Chemistry at Colorado State



University (US) with research interests in photoelectrochemical energy conversion, ultrahigh vacuum surface science, scanning probe microscopies, and inorganic fullerenes.

- Thuc-Quyen Nguyen is a Professor of Chemistry and Biochemistry at University of California at Santa Barbara (US) with research interests in the area of organic optoelectronic materials, with special emphasis on characterization of nanoscale electronic properties.
- Gang Bao is a Professor of Mathematics at Michigan State University (US) with research interests in inverse and design problems in partial differential equations, diffractive, nonlinear, near-field, and nano optics, electromagnetic and acoustic wave propagation, applied and numerical analysis.

Panel 3: Surface Chemistry, biochemistry, charge transport, and photo-processes



Yichun Liu of Northeast Normal University in China

- Jianguo Yu is a Professor of Materials Physics and Chemistry at Wuhan University of Technology (China) with research interests in semiconductor photocatalytic materials and their environmental application, nanoporous and hollow materials, nanomaterials and nano-structured materials, biomimetic synthesis, biocrystallization, and morphology control.
- Yichun Liu is a Professor of Physics at Northeast Normal University (China), with research interests in wide gap-band semiconductor materials, in particular on the growth of nano-ZnO and ZnO films, heterojunction, etc.
- Kimberly Gray is a Professor of Civil Engineering and a Professor of Chemical and Biological Engineering at Northwestern University (US), with research interests in physicochemical processes, environmental analytical chemistry, hazardous waste treatment technologies, photochemistry and radiation chemistry, and water and wastewater treatment
- Dhimiter Bello is a Professor of Health and Environment at University of Massachusetts, Lowell (US) with research interests in human health effects of exposures to nanomaterials, dose-response relationships, exposure routes and measurement issues.

Panel 4: Nano Education and Training across levels

- Yunqi Liu is a Professor of IC at the Institute of Chemistry, Chinese Academy of Science CAS (China) with research interests in design and synthesis of molecular materials, organic/polymeric light-emitting diodes, organic field-effect transistors, and preparation of carbon nanotubes and their electronic devices.
- Feiyu Kang is a Professor of Materials Science and Engineering at Tsinghua University (China) with research interests in graphite process, graphite intercalation compounds, lithium ion battery, EDLC, fuel cell, porous carbon and adsorption.
- Isiah Warner is a Professor of Analytical and Environmental Chemistry at Louisiana State University (US) with research interests in fluorescence spectroscopy, spectroscopic applications of multichannel detectors, chromatography, environmental analyses and mathematical analyses and interpretation of chemical data using chemometrics.
- RPH Chang, Professor of Materials Science and Engineering at Northwestern University (US) with research interests in carbon nanotubes, photonic crystals, advanced solar cells, nanophotonic devices in the UV optical regime, and nanowires of oxide-based materials.



Feiyu Kang of Tsinghua University

Student Poster Session

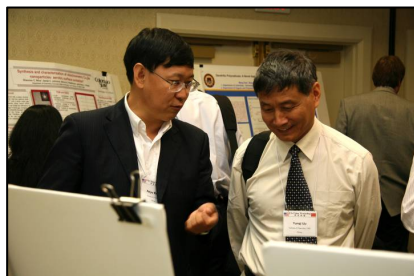
The session included the following titles from the US (please see Appendix 3 for abstracts):

- “Real-Time Measurements during Electrospinning of Polystyrene Using Raman Spectroscopy”
- “Device Physics of Bulk Heterojunction Organic Photovoltaics”
- “Nanomaterial Exposures and Biological Oxidant Damage: Towards New Exposure Metrics”
- “Biological and Environmental Transformations Engineered Nanoparticles and Impacts on Developmental Toxicity”
- “Development of New Semiconducting Polymers for High Performance Organic Solar Cells”
- “Novel Synthesis of Nanostructured Lab6 Powders for Hydrogen Storage Applications”
- “Frozen Ionic Liquid Nano- and Micro-Particles”
- “Progress in the Development of Safe Carbon Nanotubes”
- “Synthesis and Characterization of Cu₂Se Nanoparticles for Photovoltaic Applications: Aerobic Surface Oxidation”
- “The Development of Novel All Organic Dielectric Materials for Electronic and Optical Applications”



Bruce Parkinson of Colorado State and his student, Shannon Riha compare notes during the student poster session.

In addition to the above-mentioned US posters, Feiyu Kang also contributed a number of posters authored by his students at the Tsinghua University in China.



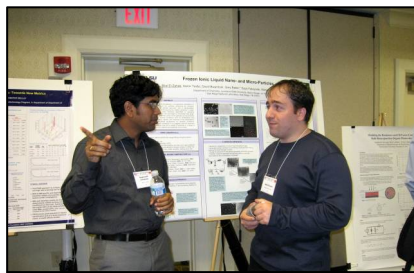
Chinese professors Feiyu Kang of Tsinghua University and Yunqi Liu of the CAS Institute of Chemistry discuss a poster.



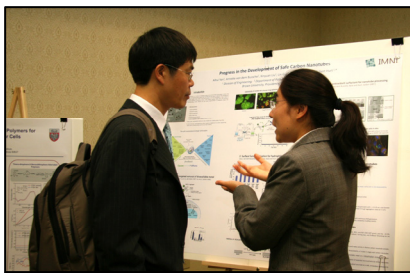
Graduate student Charusheela Ramanan of Northwestern explains her solar cell research to US and Chinese professors.



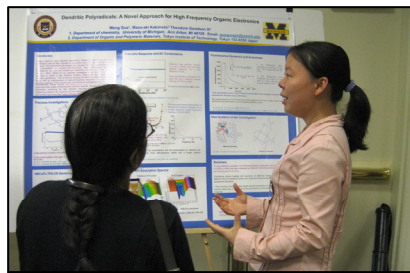
Graduate student Jon Servaites of Northwestern describes his work to Math professor Gerald Young of the University of Akron.



Graduate student Raghunath Kanakala of Alfred University and postdoc Bilal El-Zahab of Louisiana State University.



Graduate student Aihui Yan of Brown University explains her poster to Hui-Ming Cheng of the CAS Institute of Metal Research.



Graduate student Meng Guo of the University of Michigan describes her work to Uma Venkateswaran of the NSF-DMR

Presentations by Funding Agencies

NSF and NSFC representatives held an informational session describing opportunities for joint funding in the US and China. Shown clockwise below: Wei Qin of the NSFC Bureau for International Cooperation, Division of America and Atlantic; Carmen Huber of the NSF Division for Materials Research; Tingyu Li of the NSF Division of Chemistry; and Junping Wang of the NSF Division of Mathematical Sciences.



NSF-NSFC Meeting

NSF and NSFC representatives met in a closed parallel session to discuss the development of joint funding mechanisms and programs to foster US-China cooperation.

Working Group Sessions

Working Group breakout sessions were held to:

- (1) generate recommendations for improving US-China collaborations in areas of common interest and complementary strength; and
- (2) discuss and plan potential joint projects for addressing energy and environmental challenges.

Researchers and students were assigned to one of five working groups as follows:

Group 1: Advanced Solar Cell - A

- Bruce Parkinson, Colorado State University (US) –*Co-leader*
- Zhanguo Wang, Institute of Semiconductor, CAS (China) – *Co-leader*
- Geoffrey Hutchison, University of Pittsburgh (US) - *Scribe*
- Luping Yu, University of Chicago (US)
- Tobin Marks, Northwestern University (US)
- Ethan Good, Dow Corning Corporation (US)
- Qingbo Meng, Institute of Physics, CAS (China)
- Bilal El-Zahab, Louisiana State University (US)- *postdoc*
- Yongye Liang, University of Chicago (US) - *student*
- Charusheela Ramanan, Northwestern University (US) - *student*



Group 2: Advanced Solar Cell - B

- Micheal Wasielewski, Northwestern University (US) – *Co-leader*
- Yong Cao, South China University of Science & Technology (China) – *Co-leader*
- Stefan Bernhard, Princeton University (US) - *Scribe*
- Yang Yang, University of California at Los Angeles (US)
- Joseph Jerome, Northwestern University (US)
- Thuc-Quyen Nguyen, University of California at Santa Barbara (US)
- Seth Marder, Georgia Tech (US)
- Yunqi Liu, Institute of Chemistry, CAS (China)
- Meng Guo, University of Michigan (US) - *student*
- Shannon Riha, Colorado State University (US) - *student*
- John Servaites, Northwestern University (US) - *student*



Group 3: Nanomaterials and the Environment - A

- Andrew Maynard, Woodrow Wilson International Center for Scholars (US) - *Co-leader*
- Hui-Ming Cheng, Institute of Metal Research, CAS (China) – *Co-leader*
- Robert Hurt, Brown University (US) – *Scribe*
- Richard Flagan, Caltech (US)
- Feiyu Kang, Tsinghua University (China)
- Jiaguo Yu, Wuhan University of Technology (China)
- Giriprasath Gururajan University of Delaware (US) - *student*
- Paige Wicinski, University of Wisconsin (US) - *student*



Group 4: Nanomaterials and the Environment - B

- Mamadou Diallo, Caltech (US) – *Co-leader*
- Jian Xu, Institute of Chemistry, CAS (China) – *Co-leader*
- Kimberly Gray, Northwestern University (US) – *Scribe*
- Gang Bao, Michigan State University (US)
- John Rabolt, University of Delaware (US)
- Duan Weng, Tsinghua University (China)
- Shu-Feng Hsieh, University of Massachusetts, Lowell (US) - *student*
- Aihui Yan, Brown University (US) - *student*



Group 5: Novel Synthesis and Characterization of Nanostructured Materials for Environmental Health

- Isiah Warner, Louisiana State University (US) – *Co-leader*
- Jiaguo Yu, Wuhan University of Technology (China) – *Co-leader*
- Theodore Goodson, III, University of Michigan (US) – *Scribe*
- Gerald Young, University of Akron (US)
- Dhimiter Bello, University of Massachusetts, Lowell (US)
- Olivia Graeve, Alfred University (US)
- Yichun Liu, Northeast Normal University (China)
- R.P.H. Chang, Northwestern University (US)
- Raghunath Kanakala, Alfred University (US) - *student*



Special Presentation: Global E-Institute



US co-organizer R.P.H. Chang of Northwestern University

Workshop co-organizer, R.P.H. Chang of Northwestern University described a proposal to establish a jointly-funded US-China Global E-Institute.

The Institute would assemble diverse stakeholders from industry, government, and academia in the US and China to perform cross-cutting research, education, and networking at the intersection of Energy, the Environment, and the Economy.

Section 4: Group Recommendations

The five above-mentioned working groups were asked to identify:

- A. Challenges/barriers specific to US-China cooperation;
- B. Transformative approaches to jointly address global energy and environmental challenges including long-term mechanisms and “big picture” solutions; and
- C. Near-term / smaller scale solutions for enhancing US-China cooperation including improvements to existing programs and joint research projects for possible funding under existing collaborative mechanisms such as the NSF Materials World Network.

Group findings are summarized below. Working Group Guidelines appear in Appendix 5 and working group reports are available in Appendix 6.

A) Challenges

Challenges specific to US-China cooperation include:

- Distance / Travel
- Regulatory Environment (limitations on exchanges of data, materials, and property across borders, policy-related constraints on international collaboration, etc.)
- Communication (language, culture, cross-disciplinary communication)
- Interdisciplinarity (i.e., “differences in modes of cross-disciplinary operation”)
- Identifying Partnerships (i.e., “unfamiliarity with each other’s research,” and “difficulties finding suitable partners and complementary resources and facilities in China”);
- Funding (i.e., differing funding mechanisms; [lack of] cross-disciplinary funding; and [lack of] funding for targeted research.)
- Different teaching / mentoring styles and educational protocols
- Intellectual Property (government / trade issues, commercial constraints on international collaboration; export control issues; pressure to commercialize; conflict between basic and applied research, etc.)



Assistant Professor Geoffrey Hutchison of the University of Pittsburgh reports from Group 1

B) Transformative (“Big Picture”) Approaches

The groups were asked to consider new, transformative mechanisms that would help to overcome the above-mentioned barriers and foster rapid progress toward solving global energy and environmental challenges.

A key concept to emerge was that of *an overarching US-China Global Institute* to be jointly funded and managed by US and Chinese partners from the government, industry and academic sectors. By virtue of its joint ownership, such an institute would establish a seamless, sustainable environment for US-China research, education and networking and serve as a hub for global

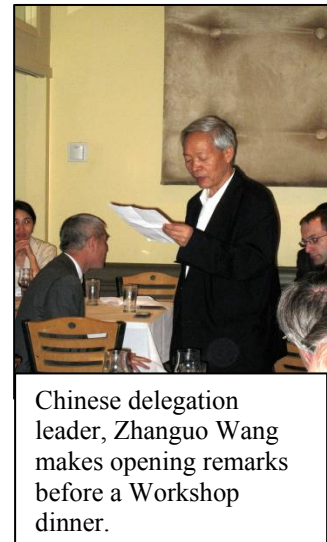
cooperation. By virtue of its large scale, it might also serve as a platform for student and faculty exchanges, a research and education clearinghouse, and a coordinating body linking nationally funded centers and institutes on both sides, creating and maintaining databases, organizing workshops, etc. By virtue of its extended lifespan, it would foster long-term partnerships, bridge language and cultural divides, and enable both countries to share resources and use their complementary capabilities to produce transformative solutions to global energy and environmental challenges. Working groups envisioned a focus on Energy, Nanomaterials and the Environment or both. A cross-cutting focus on Energy, Environment and the Economy was also mentioned. This new paradigm is a key deliverable of the Workshop, and its implementation will require the engagement of diverse stakeholders in the US and China, as described in Section 5.

C) Near-term Recommendations to Improve US-China Collaborations

Near term recommendations were made in three main areas: Networking, Education and Training, and Research. The working groups called for policy, infrastructure, and cyberinfrastructure support for their recommendations in all three of these areas. In addition, a number of joint research and networking projects were conceived for possible funding under the NSF Materials World Network or other existing funding programs.

1. Networking

- Acknowledge different work/education cultures. Emphasize human connections that will lead to substantial collaboration; Encourage longer term visits and collaborations.
- Use student interactions and exchanges to foster long-term connections. Establish a university network (complementary universities with mutual goals) as a pipeline for ongoing collaboration. Identify former US / Chinese students and postdocs who have studied in the other country, who are now faculty or administrators to lead this effort.
- Improve cyberinfrastructure to facilitate networking among potential collaborators; create databases on skills and expertise for each country, materials structure and properties, and unique complementary facilities and equipment, etc. Work with NSF and NSFC to obtain lists of researchers, researcher expertise, and key facility information.
- Encourage bilateral networking and social activities at major scientific conferences. Satellite meetings might be held slightly before or after large conferences to leverage attendance and minimize additional cost, travel and time requirements.
- Use student interactions to foster long-term connections. Strengthen student participation and organized student networking at major scientific conferences and workshops (i.e., strive for equal numbers of students and senior researchers, hold student poster sessions, organize student-led breakout sessions, matching guest students with host students, laboratory visits, cultural visits, etc.)
- Hold events in the US and China and provide sufficient travel funds for researchers and students from both sides to attend.



- Organize targeted workshops with narrower scope topics to exchange specific research results and broad topic workshops (Global Energy, Sustainable Nanotechnologies, etc.) to understand current state-of-the-art and identify future challenges.

2. Education and Training

- Train students earlier; offer more student exchange opportunities and travel grants.
- Encourage long-term student and faculty exchanges; remove visa and other barriers
- Equalize ratio of exchange students - encourage and provide mechanisms for more US students to study abroad.
- Use student exchanges to:
 - promote social interactions and long-term relationships
 - address cultural differences and language barriers
 - share approaches for solving pressing global problems
 - facilitate discussion on emerging areas of research
 - fuel bottom-up research collaborations
- Provide early career leadership training; offer students opportunities to lead research discussions, organize workshops, plan collaborative projects, write joint proposals, etc.
- Adapt and improve existing programs for use with US and Chinese students. For example, International Research Experience for Undergraduates (REU) with cultural Experience, NSF-US-China International Graduate Fellowship, Global School for Advanced Studies (global leadership training), etc.
- Establish remote tutoring labs and remote instruction (distance learning), such as iLabs, which is currently being implemented at Northwestern and MIT through NSF



Graduate students Meng Guo and Shannon Riha

3. Research Collaborations

- Identify focus areas for collaboration. Good opportunities exist to integrate material synthesis, structure, function, and theory, computation in US and China.
- Keep focus on fundamental scientific and technological grand challenges across disciplines and national boundaries. Keep IP and commercialization in perspective.
- Start with simple, bottom-up proposals with timely evaluation mechanisms to allow for effective initiation and continuation. Provide seed funding and travel grants to plan projects.
- Develop shared resources (materials properties database, shared technologies for detection and measurement, etc.)
- Identify shared facilities such as the Advanced Photon Source in US; identify gaps in complementary user facilities (e.g., neutron/x-ray sources, etc.) that are available for collaborative research

4. Potential Areas for Collaboration

Joint research and networking projects were conceived for possible funding under the NSF Materials World Network or other existing funding programs. Groups were asked to provide

project rationale, goals, required expertise and potential participating institutions in US and China, collaboration structure, complementary facilities and capabilities, anticipated outcomes, broader impact including integration of research with education, budget considerations, and action items. Thumbnail descriptions are given below. See Appendix 6 for full descriptions.

Group 1 – Advanced Solar Cells –A

- “Understanding and Controlling Organic Phase Segregation in Bulk Heterojunction Photovoltaic Materials.” Goals to include: Understanding issues affecting morphology and phase separation at the nanoscale using advanced characterization techniques; understanding how surface area and phase segregation affect carrier generation and loss mechanisms; developing predictive theoretical / computational models of nanoscale and mesoscale phase evolution; using this information to design synthetic modifications to donor and acceptor components with desired morphologies.
- “Overcoming Charge Transport Limitations in Organic Bulk-Heterojunction Photovoltaics.” goals to include: demonstrating, understanding and controlling singlet exciton fission and multi-exciton generation; understanding and controlling 2D charge transport; characterizing and understanding all loss mechanisms (electrical, optical, etc.) at contacts and donor/acceptor interfaces; using this information to rationally design novel device architectures with improved efficiencies.
- “Nanostructured Inorganic/Organic Hybrid Photovoltaic Devices” with goals to include: integrating organic photovoltaic materials into nanostructured inorganic devices; pairing of optimal organic photovoltaic materials and appropriate nanostructured inorganic semiconductor; introduction of surface functionalization at organic/inorganic interface to control wetting, charge blocking, adhesion/cohesion, and manipulate surface dipoles and charge injection; and use of nanostructured inorganic material to control organic morphology and microscopic and long-range order.

Group 2 - Advanced Solar Cells –B

- “Novel Functional Materials for Solar Energy Conversion” including: judicious control of electronic and charge-transport properties; easily processable materials with consistent properties and purity; nontoxic materials synthesized from abundant elements; high photo and redox stability (mixed inorganic and organic); and modeling of relevant properties in solution and in the solid state.
- Device Engineering, including: methodology to investigate and control the factors that influence open circuit voltage, short circuit current, and fill factor; development of novel techniques for understanding the interplay of material workfunctions, HOMO-LUMO gap and position in devices; and correlation of the morphology of interfaces with their observed charge transfer rates.

Group 3 – Nanomaterials and the Environment – A

- Nanomaterial liberation, detection and quantification focus on nanomaterials in environmental samples (air, soils, water, sediments, surfaces) and products. Three elements: detection methodologies, physics of nanomaterial release, characterization of nanomaterials

in all relevant environmental media. Priorities: air in workplace, contact exposure (workplace and consumer use)

- Green Nanomanufacturing, focusing on the scientific issues arising in the systematic design of environmentally benign nanoproducts and nanoprocesses. Projects could center on specific material case studies, and consider: Process engineering science for nanofabrication; Manufacturing safety; Nano-pollution control and prevention (replacement of hazardous solvents, intermediates, product toxicity control); Life-cycle analysis (incl. carbon footprint, impact on water resources)
- Series of joint US-China workshops on Sustainable Development of Nanotechnologies that would: 1) focus on one materials class (e.g. carbons) per meeting or per session; 2) deal with full range of issues, including exposure, toxicity, life-cycle analysis, and safe design strategies, 3) involve specific “stakeholders” in those materials (experts in synthesis, device development, environmental science, and health impacts) can exchange detailed scientific information and reach concrete conclusions about prospects and research directions
- An International Institute for Sustainable Nanotechnology Development as a world-wide hub of exchange and cooperation, for potential funding under the NSF IMI program.

Group 4 - Nanomaterials and the Environment – B

- “Membranes from Polymeric Nanofibers” Goals: Develop structure-properties relationships that can be used to guide the design fabrication of novel nanofiber-based membranes for water treatment and gas separation
- “Structure, Processing and Properties of Polymer Nanofibers for Light Sensing, Sound Absorbance and Filtration” Goals: Understand the relationship between the structure (molecular, crystal and morphological), processing and properties of polymer nanofibers so as to be able to optimize their performance in sensing, absorbance and filtration applications. Develop a room-temperature electrospinning process that allows the incorporation of “guest” molecules into the nanofibers with a subsequent migration to the surface so as to sequester contaminants, absorb/reflect light or reduce sound.
- “Transparent Surface Coating with Nanostructure and Anti-reflection Properties” Goals: Based on the nano-structure, the light transmittance of the coated glass slide is up to 92%~97% in the visible light range (390~780nm) and 95% ~ 97 % in the major visible light range (460~750). That above-mentioned indicated that the as-prepared film can improve the light transmittance of substrate material. Another objective to develop computational models and tools for systematic designs and modeling of the intended nano structures.

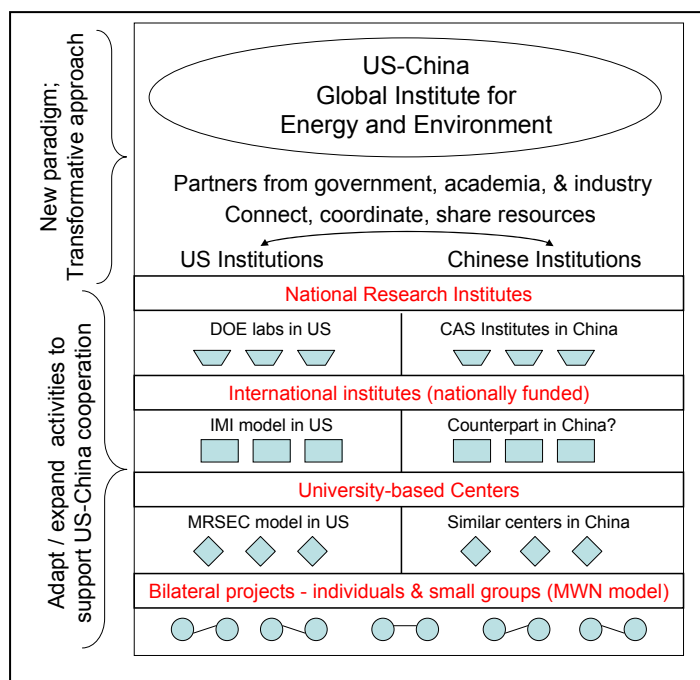
Group 5 – Novel Synthesis and Characterization for Environmental Health

- “Non-template Self-transformation Fabrication of Hollow Inorganic Microspheres and Their Application in Water and Air Purification” Potential collaboration with engineer/materials science to carry out the fabrication of a real device to test the purification procedure.
- “Investigations of High Dielectric Constant Effects in Pthalocyanine Systems” Goals: obtain a set of parameters related to the functionalization of pthalocyanine nanomaterials and dielectric properties and to use a number of spectroscopic topics to probe the mechanism of electron and energy transfer in these materials.

Section 5: Implementation Strategy

The organizers propose the following implementation strategy based on their review of group recommendations. Feedback and leadership from the community is welcome.

Adapting or Expanding Existing Mechanisms: Most Workshop recommendations suggest improvements and adaptations to collaboration mechanisms that already exist in the US and China, as illustrated in the figure below. For example, a number of bilateral research projects involving individual researchers or small groups of researchers were developed for potential funding under the Materials World Network (MWN) joint funding framework. Moving up the scale, university-based research centers (such as MRSEC and NSEC) will find numerous suggestions for improving their collaborative research and graduate and undergraduate education



programs. Many of these centers already offer international REU and graduate exchanges with China. International institutes (such as the IMI model) and national research institutes such as (DOE labs in the US and CAS institutes in China) will also find recommendations for networking, exchange programs and collaborative research with China.

Implementation: The organizers call on the participants of this first Workshop to take the lead in implementing these suggestions at their respective institutions and to request joint funding for the collaborative projects that they developed. The Workshop cyberinfrastructure remains available for ongoing discussions and project development (www.materialsworld.net).

New, transformative paradigm: Participants also suggested a new mechanism for higher-level cooperation: a US-China Global Institute. Such a body would be jointly owned and managed by US and Chinese partners and connect national and international programs on both sides to create a seamless, sustainable collaborative environment in which US and Chinese partners could pursue transformative solutions to global energy and environmental challenges.

Implementation: The implementation of this paradigm will require the engagement of stakeholders in government, academia and industry. Government partners will need to establish a sustainable joint funding structure and facilitate shared access to national facilities. Academic partners will need to bring research expertise, educational programs and infrastructures, and laboratory facilities. Partners from industry will need to contribute guidance in technology development, sponsorship, and opportunities for human resource development. The second Workshop in China will be an excellent opportunity for implementation. Meanwhile, the organizers plan to launch quarterly online discussions involving the participants and various other stakeholders. Based on these discussions, they will determine the need for a formal planning event.

Section 6: Conclusions

The Workshop successfully met its goals, thanks in great part to the careful selection of diverse participants from the US and China who contributed diligently to the discussions and group reporting processes. Both sides agreed to expand student participation in future workshops and equalize representation from both sides.

The Workshop was especially timely in the current economic climate because it discussed the consolidation of resources and expertise from two of the largest world economies and the sustainable advancement of economic growth through solar cell and environmental technologies. The event had the added benefit of assembling US researchers and their students from across the country to forge professional connections and learn about relevant research being performed domestically and in China. Strong representation from the NSF and the NSFC also created an opportunity for discussions of programmatic infrastructures to support US-China collaboration.

The Workshop was an opportunity to consider near-term improvements to existing programs and mechanisms and long-term “big picture” requirements for solving urgent global energy and environmental challenges through transformative approaches and new levels of cooperation. Key deliverables included:

- Improved understanding of complementary expertise and resources in both countries
- Suggestions for improving collaborative research, education, and networking in the near term and the long term including research databases, cyberinfrastructure, new workshop series, expanded student exchanges, etc.
- Specific improvements to existing education programs such as NSF REU, Graduate Fellowships, etc.
- A list of bilateral research projects for potential joint funding under the NSF Materials World Network framework
- A new collaboration paradigm - a jointly funded and operated US-China institute that would provide a sustainable, seamless environment for collaborative research, education and networking.

It is hoped that the participants from this first Workshop will lead efforts to implement these recommendations by working with their respective universities, labs, government agencies, students and colleagues. The community-based cyberinfrastructure remains available to support their ongoing discussions (www.materialsworld.net). The Workshop organizers plan to launch quarterly discussions in order to maintain momentum and engagement between Workshops.

The organizers trust that the recommendations and project outlines produced at this workshop will be a useful resource for the funding agencies in their ongoing efforts to support US-China cooperation in the critical global challenge areas of energy and the environment.

The second workshop in this series will be held in China in October 2009.

Appendix 1: Participant List

From China

Last Name	First Name	Title	Affiliation	Role
Cao	Yong	Institute of Polymer Optoelectronic Materials and Devices,	South China University of Science & Technology	Researcher
Che	Chengwei	Professor, Director, Division of Metal Material, Bureau of Engineering and Materials	National Natural Science Foundation of China	Observer
Chen	Kexin	Professor, Director, Division of Ceramics Material, Bureau of Engineering and Material, NSFC	National Natural Science Foundation of China	Observer
Cheng	Hui-Ming	Professor, Head - Research Division, Institute of Metal Research, CAS	Institute of Metal Research, CAS	Researcher
Gao	Ruiping	Professor, Deputy Director-General, Bureau of Engineering and Materials	National Natural Science Foundation of China	Observer and Vice Chinese Delegation Leader
Kang	Feiyu	Professor, Dean, New Carbon Materials Laboratory	Tsinghua University	Researcher
Liu	Yichun	Professor of Condensed Matter Physics	Northeast Normal University	Researcher
Liu	Yunqi	Professor - Physical Chemistry, CAS Key Laboratory of Organic Solids	Institute of Chemistry, CAS	Researcher
Meng	Qingbo	Professor - Condensed Matter Physics (surface Physics)	Institute of Physics, CAS	Researcher
Wang	Zhanguo	Professor and Chair of SIMC-XIII-2004, International Advisory Committee Member	Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, CAS	Researcher and Chinese Delegation Leader
Wei	Qin	Program Officer, Division of America and Atlantic, Bureau of International Cooperation, NSFC	National Natural Science Foundation of China	Observer
Weng	Duan	Professor of Materials Science and Engineering	Tsinghua University	Researcher and Co-organizer
Xu	Jian	Professor, Research Professor - Polymer Chemistry & Physics	Institute of Chemistry, CAS	Researcher
Yu	Jiaguo	Professor of Materials Physics and Chemistry, State Key Laboratory of Advanced Technology for Materials Synthesis and Processing	Wuhan University of Technology	Researcher

From the US

Last Name	First Name	Title	Affiliation	Role
Bao	Gang	Professor of Mathematics	Michigan State University	Researcher
Bello	Dhimiter	Professor of Work Environment	University of Massachusetts, Lowell	Researcher
Bernhard	Stefan	Professor of Chemistry	Princeton University	Researcher
Chang	R.P.H.	Professor of Materials Science and Engineering	Northwestern University	Researcher and Co-organizer
Diallo	Mamadou	Director of Molecular Environmental Technology, Materials & Process Simulation Center	California Institute of Technology	Researcher
Echegoyen	Luis	Director, Chemistry Division, National Science Foundation	National Science Foundation	Observer
El-Zahab	Bilal	Postdoctoral Fellow, Chemistry	Louisiana State University	Student
Flagan	Richard	Executive Officer of Chemical Engineering, Professor of Chemical Engineering and Professor of Environmental Science & Engineering	California Institute of Technology	Researcher
Good	Ethan A.		Dow Corning Corporation	Researcher
Goodson	Theodore	Professor of Chemistry	University of Michigan	Researcher
Graeve	Olivia	Associate Professor, Materials Science and Engineering	Alfred University	Researcher
Gray	Kimberly	Professor of Civil and Environmental Engineering	Northwestern University	Researcher
Guo	Meng	Graduate Student, Chemistry	University of Michigan	Student
Gururajan	Giriprasath	Graduate Student, Materials Science and Engineering	University of Delaware	Student
Hsieh	Shu-Feng	Graduate Student, Work Environment	University of Massachusetts, Lowell	Student
Huber	Carmen	Acting Executive Officer, Division of Materials Research	National Science Foundation	Observer
Hupp	Joseph	Chair, Chemistry Department	Northwestern University	Observer
Hurt	Robert	Professor of Engineering	Brown University	Researcher
Hutchison	Geoffrey	Professor of Chemistry	University of Pittsburgh	Researcher
Jerome	Joseph	Professor of Mathematics	Northwestern University	Observer
Kafafi	Zakya	Director, Division of Materials Research	National Science Foundation	Observer
Kanakala	Raghunath	Graduate Student, Materials Science and Engineering	Alfred University	Student
Li	Tingyu	CHE Division of Chemistry	National Science Foundation	Observer
Liang	Yongye	Graduate Student, Chemistry	University of Chicago	Student

From the US, continued

Last Name	First Name	Title	Affiliation	Role
Lueptow	Richard	Senior Associate Dean for Operations and Research, McCormick School	Northwestern University	Observer
Marder	Seth	Professor; Director of the Center for Organic Photonics and Electronics (COPE)	Georgia Institute of Technology	Researcher
Marks	Tobin	Professor of Catalytic Chemistry & Materials Science and Engineering	Northwestern University	Researcher
Maynard	Andrew	Chief Science Advisor	Woodrow Wilson International Center for Scholars	Researcher
Miksis	Michael	Chair, Engineering Sciences and Applied Mathematics	Northwestern University	Observer
Nguyen	Thuc-Quyen	Professor of Chemistry	University of California at Santa Barbara	Researcher
Parkinson	Bruce	Professor of Chemistry	Colorado State University	Researcher
Rabolt	John	Chair, Materials Science and Engineering	University of Delaware	Researcher
Ramanan	Charusheela	Graduate Student, Chemistry	Northwestern University	Student
Riha	Shannon	Graduate Student, Chemistry	Colorado State University	Student
Servaites	Jonathan	Graduate Student, Materials Science and Engineering	Northwestern University	Student
Venkateswaran	Uma	Program Director, Office of Special Programs Division of Materials Research	National Science Foundation	Observer
Walsh	Jay	Vice President for Research	Northwestern University	Observer
Wang	Junping	Program Director, Division of Mathematical Sciences	National Science Foundation	Observer
Warner	Isiah M.	Professor of Chemistry; Vice Chancellor	Louisiana State University	Researcher
Wasielowski	Michael	Professor of Chemistry	Northwestern University	Researcher
Wiecinski	Paige	Graduate Student, Civil and Environmental Engineering	University of Wisconsin	Student
Yan	Aihui	Graduate Student, Engineering	Brown University	Student
Yang	Yang	Professor of Materials Science and Engineering	University of California at Los Angeles	Researcher
Ying	Charles	Division of Materials Research	National Science Foundation	Observer
Young	Gerald	Professor of Mathematics	University of Akron	Researcher
Yu	Luping	Professor of Chemistry	University of Chicago	Researcher

Appendix 2: Program

Monday, September 22

Workshop Goal 1: Identify potential research areas/topics to address shared energy and environmental challenges facing the US and China.

Opening Remarks

8:00 - 8:30 Co-organizers, RPH Chang (US) and Duan Weng (China)
NSF Division Directors - Zakya Kafafi (DMR) and Luis Echegoyen (Chemistry);
NSFC Bureau Deputy Director - Ruiping Gao (Engineering and Materials)

Speaker Sessions

Session 1: Nanomaterials and the Environment

Session Chair: Andrew Maynard, Woodrow Wilson International Center for Scholars (US)

8:30- 9:00 Duan Weng, Tsinghua University (China)
9:00-9:30 Richard Flagan, California Institute of Technology (US)
9:30-9:45 Discussion

Session 2: Advanced Solar Cells

Session Chair: Luping Yu, University of Chicago (US)
10:00-10:30 Yang Yang, University of California at Los Angeles (US)
10:30-11:00 Yong Cao, South China University of Science & Technology (China)
11:00 Discussion

Cross-Cutting Panels

Each panelist will briefly outline his/her related research *and* suggest a list of important open questions relating to advanced solar cells, environmental health/protection, and/or novel nanostructured materials, followed by open discussion. Ideas generated during the panels will inform working group discussions on Tuesday.

Panel 1: Nanomaterials Synthesis (particles, rods, hollow structures, etc)

Moderator: Zhanguo Wang, Institute of Semiconductor, CAS (China)

11:15- 12:15

- Hui-Ming Cheng, Institute of Metal Research, CAS (China)
- Jian Xu, Institute of Chemistry, CAS (China)
- Olivia Graeve, Alfred University (US)
- Stefan Bernhard, Princeton University (US)

Lunch

Panel 2: Nano Characterization Techniques (electron, photon, and ion spectroscopies)

Moderator: Yong Cao, South China University of Science & Technology (China)

1:45-2:45

- Zhanguo Wang, Institute of Semiconductor, CAS (China)
- Yunqi Liu, Institute of Chemistry, Chinese Academy of Science (China)
- Bruce Parkinson, Colorado State University (US)
- Thuc-Quyen Nguyen, UC Santa Barbara (US)
- Gang Bao, Michigan State University (US)

Panel 3: Surface Chemistry, biochemistry, charge transport, and photo-processes

Moderator: Tobin Marks, Northwestern University (US)

2:45-3:45

- Jiaguo Yu, Wuhan University of Technology (China)
- Yichun Liu, Northeast Normal University (China)
- Kimberly Gray, Northwestern University (US)
- Dhimiter Bello, University of Massachusetts Lowell (US)

Panel 4: Nano Education and Training across levels (pre-college, college, and graduate)

Moderator: Ethan Good, Dow Corning (US)

4:00-5:00

- Yunqi Liu, Institute of Chemistry, Chinese Academy of Science (China)
- Feiyu Kang, Tsinghua University (China)
- Isiah Warner, Louisiana State University (US)
- RPH Chang, Northwestern University (US)

Poster Session

5:00-6:00

Tuesday, September 23

Workshop Goal 2: Generate recommendations for addressing these challenges together, including potential jointly funded research projects between the US and China.

Workshop Goal 3: Establish active US-China working groups in these areas, as part of the Materials World Network.

Joint Funding Mechanisms

8:30 – 10:00

NSF and NSFC officials describe mechanisms for joint funding, followed by Q&A

Working Group Instructions

10:00-10:15

*****Group Photos*****

Working Group Breakout Sessions

Five working groups will generate recommendations and discuss / plan potential joint projects.

- Group 1: Advanced Solar Cell - A *(Northshore A)*
- Group 2: Advanced Solar Cell - B *(Northshore B&C)*
- Group 3: Nanomaterials and the Environment - A *(Lakeshore A)*
- Group 4: Nanomaterials and the Environment - B *(Lakeshore B)*
- Group 5: Novel Synthesis and Characterization of Nanostructured Materials for Environmental Health *(Grill Room)*

Breakout Session 1

*****Closed NSF-NSFC Meeting ***** *(Boardroom)*

10:30-12:00

*****Lunch*****

Breakout Session 2

*****Closed NSF-NSFC Meeting ***** (Boardroom)

1:30-3:00

Breakout Session 3

3:15-4:30

Group Reports and Discussion

4:30-5:30

Group Summaries (5 minutes per group), followed by discussion

*****Dinner hosted by Northwestern University*****

(Stained Glass Restaurant 1735 Benson Ave. Evanston)

7:00

Wednesday, September 24

Workshop Goal 2: Generate recommendations for addressing these challenges together, including potential jointly funded research projects between the US and China.

Workshop Goal 3: Establish active US-China working groups in these areas, as part of the Materials World Network.

Breakout Session 4

9:00-10:00

Working groups finalize priorities for future implementation.

Joint Group Discussions

10:00-11:00

Groups come together to discuss priorities and consider potential implementation.

Preparation of Workshop Report / Participant Survey

11:00-11:30

Leaders and Scribes distill priorities and combine their group reports into a single workshop report. Submit reports and surveys.

*****Lunch*****

Adjourn Workshop

Appendix 3: Abstracts for Talks and Posters

TALK 1: STATE-IN-ART OF ECOMATERIALS IN CHINA

Duan Weng*, Lei Wang, Rui Ran, Xiaodong Wu

Department of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

Materials are one of the most important supports for modern society. As a sustainable century, the sustainable development of society and economics in the 21st century is based on the coordinativity with natural resource and environmental endurance. It is very important to keep the balance among resource, energy and ecological environment during the production, application and disposal of materials. As a new boundary science, the ecomaterials is just created for the purpose. In this presentation, some consideration on the fundamental of ecomaterials will be demonstrated such as the goal and content of ecomaterials. The definition and characteristics of ecomaterials are described, including higher eco-efficiency, no poisonous, lower emission and higher recycling. Three main types of ecomaterials are introduced, including environmental engineering materials, environment-friendly materials and environmental functional materials. About the key technologies of ecomaterials, the element replacement in the lead-free revolution is presented as an example. In the theoretic research on ecomaterials, the methodology of life cycle assessment is discussed. In the end, prospects for future progress in the development of ecomaterials are also forecasted. **Keywords:** ecomaterials, environmental engineering materials, environmental functional materials, environment-friendly materials, life cycle assessment (LCA), environmental Impact, resource productivity

TALK 2: NANOPARTICLES IN THE ENVIRONMENT

Richard C. Flagan

Chemical Engineering and Environmental Science and Engineering

California Institute of Technology 210-41

Pasadena, CA 91125

Little is known of the risks that nanotechnology may pose to the environment or to workers in the nanotechnology industries. The limited information available indicates that the fine structures that impart special properties to the products of nanotechnology do affect their health and environmental consequences. Important lessons can be drawn from exposures to nanostructures from conventional pollution sources and occupational exposures. Recent epidemiological studies reveal that PM_{2.5} exposures, i.e., the mass concentration of airborne particles smaller than 2.5 μ m diameter, are statistically associated with increased morbidity and mortality, and there is a growing body of evidence that nanoparticles exhibit even stronger effects, and that those effects are highly localized near sources such as busy freeways and highways.

The risks posed by manufactured nanoparticles and other nanotechnology products are not quantifiable today because little is known about exposures. Instruments exist that can measure the physical and chemical properties of airborne particles throughout the nanometer size domain, and even into the subnanometer regime. Most of the instruments in use today are large, complex, and expensive, making them impractical for routine environmental and exposure measurements. New instruments are, however, being developed that show promise for routine measurements of exposure to airborne nanoparticles and even for use as personal monitors.

Measurements of nanoparticles in water and on surfaces are much more difficult than in air. Nanoparticle suspensions may be characterized using dynamic light scattering, but the method provides limited and biased information since it relies on light scattering from a cloud of nanoparticles. Electron and scanning probe microscopies can provide quantitative measurements, but at high cost and after long sample processing times. This talk will discuss some of the approaches that are being explored to understand environmental nanoparticle concentrations in both air and water.

TALK 3: HIGH PERFORMANCE POLYMER SOLAR CELLS FOR RENEWABLE ENERGY

Yang Yang

Department of Materials Science and Engineering,
University of California at Los Angeles
Los Angeles, CA 90095-1595

In this presentation, recent progress in organic solar cell research at UCLA will be reported. We have discovered that by manipulation of polymer morphology, the efficiency of polymer solar cell can be dramatically improved. The morphology can be manipulated by either thermal, by solvent annealing, and by additives. In parallel, an effort to enhance the PV cell performance by adding the quantum dots has resulted surprised results.

The QDs completely quench the photovoltaic effect, but produce a high gain photo-conductivity in the reversed bias condition. This discovery paves a way for future high performance polymer detectors.

TALK 4: STUDIES AND RECENT PROGRESS OF POLYMER BULK-HETEROJUNCTION PHOTOVOLTAIC DEVICES

Yong Cao

Institute of Polymer Optoelectronic Materials and Devices,
South China University of Technology, Guangzhou, 510640, P.R.China

Photovoltaic devices using organic and polymer materials have attracted considerable interest recent years. Among varieties of concepts proposed for organic/polymer solar cells, the polymer bulk heterojunction solar cell is one of the most attractive and promising approaches. After brief introduction of mechanism of polymer heterojunction solar cells and recent progress worldwide and in the Mainland of China, we will concentrate on recent studies and progress performed at SCUT group. This will include our research in the following aspects:

1. Synthesis and device performance of new donor and acceptor materials
2. Nanomaterials synthesis for polymer/inorganic semiconductor hybrid photovoltaic devices
3. Morphology control and interface optimization
4. Efforts towards to all-printable optoelectronic device

The limiting factors for such type of devices and future perspective for solution processable, large area polymer solar cell will be discussed.

POSTER 1: THE DEVELOPMENT OF NOVEL ALL ORGANIC DIELECTRIC MATERIALS FOR ELECTRONIC AND OPTICAL APPLICATIONS

Meng Guo^a and Theodore Goodson III^a

^aDepartment of Chemistry, University of Michigan, 930 N. University, Ann Arbor, MI, 48109

Organic materials are important for a variety of optical and electronic applications. New materials which show intermolecular excitations within a macromolecular framework may be useful for enhanced effects important to light harvesting, nonlinear optics, quantum optics, and electronic applications^[1-5]. In this presentation a novel approach of utilizing all organic materials for the purpose of high energy density at relatively high frequencies (> 1 MHz) will be demonstrated. These properties in an all organic material are essential for the advancement of a low-cost, compact electronic system. These materials may also be used for high energy and power capacitive storage applications. The use of branched structures for this purpose will be presented. The electronic and optical properties of a number of novel branched systems will be described. The use of measurements such as capacitance, AC conductance, steady-state absorption and emission, time-of-flight mobility, electron magnetic resonance, ultra-fast time-resolved fluorescence and transient absorption spectroscopy will be presented for the complete characterization of the dendrimer materials. A novel hyper-branched copper phthalocyanine dendrimer with a high dielectric constant of ~ 46 at 1 MHz was found^[6, 7]. This novel material is well suited for applications as gate dielectrics for organic transistors. By comparing the properties using these techniques of a number of different branched delocalized systems we have obtained new insight in the design of superior dielectric materials^[8].

- (1) Goodson III, T. *Acc. Chem. Res.* **2005**, 38 (2), 99-107.
- (2) Zhang, Q. M.; Li, H. F.; Poh, M.; Xia, F.; Cheng, Z. Y.; Xu, H. S.; Huang, C. *Nature* **2002**, 419, 284.
- (3) Yan, X. Z.; Goodson III, T. *Phys. Chem. B*, **2006**, 110, 14667-14672.
- (4) He, Z.; ISHIZUKA, T.; Jiang, D. L. *Polym. J.* **2007**, 39 (9), 889-922.
- (5) Chu, B. J.; Zhou, X.; Ren, K. L.; Neese, B.; Lin, M. R.; Wang, Q.; Bauer, F.; Zhang, Q. M. *Science* **2006**, 334-336.
- (6) Guo, M.; Yan, X.Z.; Young, K.; Teruaki, H.; Kakimoto, M.A.; Goodson III, T. *J. Am. Chem. Soc.* **2006**, 128, 14820.
- (7) Guo, M.; Yan X. Z.; Goodson III, T. *Adv. Mater.* **2008**, ASAP.
- (8) Guo, M.; Kakimoto, M.A.; Goodson III, T. *J. Am. Chem. Soc.* **2008**, submitted.

POSTER 2: SYNTHESIS AND CHARACTERIZATION OF CU₂SE NANOPARTICLES FOR PHOTOVOLTAIC APPLICATIONS: AEROBIC SURFACE OXIDATION

Shannon C. Riha, Derek C. Johnson, Bruce A. Parkinson, and Amy L. Prieto

Chemistry Department, Colorado State University
Fort Collins, CO 80523

Copper selenide thin films and nanoparticles have received increasing attention with their potential applications in high efficiency solar cells,^{1,2} photovoltaic devices,³ as well as numerous other applications. The wide array of possible electric and optoelectric applications for copper selenide stem from the plethora of stoichiometric (CuSe, Cu₂Se, Cu₃Se₂, CuSe₂) and nonstoichiometric (Cu_{2-x}Se) compositions; thereby leading to variations in the crystal structure, band gap energies, and oxidation state of the Cu and Se.

Copper (I) selenide is a p-type semiconductor with a widely varying indirect band gap of 1.1-1.5 eV and a direct band gap of 2.0-2.3 eV.⁴ The indirect band gap lies near the optimal value for solar cell applications when exhibiting semiconductor behavior. Some researchers, however, report ohmic type behavior, which, in turn, can hinder the efficiency of the solar cell. We have therefore synthesized Cu₂Se nanoparticles and tracked its stability through X-ray photoelectron spectroscopy and X-ray diffraction studies, as well as monitored the electronic properties of a nanoparticle thin film as a function of air exposure through current-voltage measurements. Upon exposing the nanoparticles to air, gradual oxidation of Cu⁺¹ and Se⁻² occurs immediately, ultimately leading to a change in crystal structure. The electronic properties of Cu₂Se nanoparticle thin film parallel the observed oxidation and change in crystal structure. As illustrated in Figure 1, Cu₂Se exhibits semiconducting behavior under an inert atmosphere. However, as the stoichiometry and crystal structure evolve as a result of oxygen exposure, the semiconductor response is quickly converted to an ohmic one within hours of air exposure.

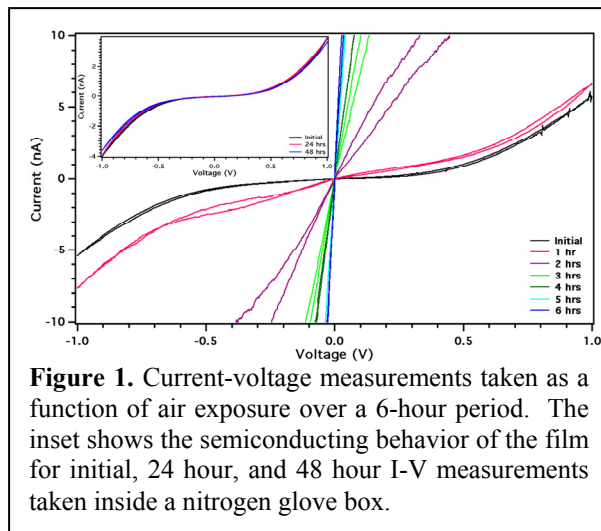


Figure 1. Current-voltage measurements taken as a function of air exposure over a 6-hour period. The inset shows the semiconducting behavior of the film for initial, 24 hour, and 48 hour I-V measurements taken inside a nitrogen glove box.

The current focus is the design and characterization—through current density-voltage and photocurrent studies—of a Cu₂Se nanoparticle thin film heterojunction solar cell. During that process, spectrophotometer measurements of the unoxidized particles will also be conducted to confirm the indirect and direct band gap energies. These measurements are crucial, as there is some discrepancy in the literature regarding the direct band gap, which can possibly be attributed to the formation of a surface copper oxide.

1. Chen, W. S.; Stewart, J. M.; Mickelsen, R. A. *Applied Physics Letters* 1985, 46, (11), 1095-1097.
2. Okimura, H.; Matsumae, T.; Makabe, R. *Thin Solid Films* 1980, 71, (1), 53-59.
3. Mane, R. S.; Kajve, S. P.; Lokhande, C. D.; Han, S. H. *Vacuum* 2006, 80, (6), 631-635.
4. Pathan, H. M.; Lokhande, C. D.; Amalnerkar, D. P.; Seth, T. *Applied Surface Science* 2003, 211, (1-4), 48-56.

POSTER 3: PROGRESS IN THE DEVELOPMENT OF SAFE CARBON NANOTUBES

Aihui Yan, Annette von Dem Bussche, Xinyuan Liu, Agnes Kane, and Robert Hurt
 Department of Engineering, Brown University
 Providence RI 02912

Carbon nanotubes are key enabling components in a number of emerging energy and environmental technologies. Concern has been raised about potential adverse health effects, and several recent studies have reported the early signs of asbestos-like pathogenicity in mice, at least for high nanotube doses. Others studies report nanotubes to be biocompatible, and this inconsistency is due in part to differences in nanotube composition (comprising tubular graphene, amorphous carbon, metal catalyst residues, defect sites, and functional groups). This material complexity makes nanotoxicology studies difficult, but also opens opportunities to intelligently design and formulate CNTs for improved safety.

Here we report on our laboratory's efforts to improve nanotube biocompatibility through processing. First, new assays have been developed to determine the "bioavailable" fraction of nanotube metal (Ni, Fe, Y) that participates in known toxicity mechanisms. Treatment with a non-oxidizing acid followed by extensive water washing is recommended as a procedure to remove the bioavailable portion of CNT metal. The acid washed carbon nanotubes showed no observable metal mobilization over two months in a flowing intracellular simulant fluid (pH 4.5) supplemented with ascorbate, H₂O₂, and Fe²⁺ for continuous generation of reactive oxygen species. Second, we report that unfunctionalized, hydrophobic nanotubes cause apparent toxicity by adsorbing folic acid from cell culture medium. This mechanism can be suppressed by chemical addition of -SO₃H groups based on diazonium chemistry. Third, a new water-soluble vitamin-E based antioxidant surfactant, TPGS, shows promise for the "green" processing of nanotubes. Our preliminary cell studies show that the presence of TPGS coating on nanotubes reduces oxidative stress caused by Fe-containing MWCNTs taken up by AML12 hepatocytes. Finally, the potential for length control to avoid asbestos-like mechanisms, and the overall prospects for safe nanotube design will be discussed.

POSTER 4: FROZEN IONIC LIQUID NANO- AND MICRO-PARTICLES

Bilal El-Zahab, Aaron Tesfai, David Bwambok, Gary Baker,† Mark Lowry, Sayo Fakayode, and Isiah Warner

Chemistry Department, Louisiana State University, Baton Rouge, LA

† Oak Ridge National Laboratory, Oak Ridge, TN

We report on the first method leading to homogeneous populations of stable, frozen ionic liquid (IL) particles employing an emulsion templating approach. The employed melt-emulsion-quench approach yields spherical or quasi-spherical particles with mean diameters dependent on the droplet size of the internal phase, allowing control in the nanometer to micrometer size range. The size, shape, and uniformity control of the particles can be achieved by varying the temperature, emulsifier, homogenizing force and concentrations. The ease, rapidity, and simplicity of the preparation, requiring neither specialized equipments nor extreme conditions, coupled with the tunable properties of ILs suggests that this approach to solid-state IL particles may find a wealth of potential in a range of areas, particularly in the material and analytical communities. The authors acknowledge the Nation Science Foundation (NSF) and the National Institutes of Health (NIH) for their financial support.

POSTER 5: INCORPORATING PERYLENE DIMIDE DERIVATIVES INTO ORGANIC PHOTOVOLTAICS

Charusheela Ramanan, Tobin J. Marks*, Michael R. Wasielewski*

Department of Chemistry, Northwestern University, Evanston, IL

In the quest for cost-effective materials for efficient organic photovoltaic devices, perylene diimide (PDI) compounds have long been of interest due to their high extinction coefficients, low cost, reliable behavior as electron acceptors, and ease of synthetic manipulation. One difficulty in incorporating these compounds, however, is that they are unsuitable for bulk heterojunction style solution processing in conjunction with well-known conductive polymers such as poly(3-hexyl)-thiophene (P3HT). This difficulty is in part attributed to the tendency of the perylene core

to form π - π aggregates in films. During solution processing, this aggregation leads to large trapping sites in the active layer. This work seeks to synthesize new PDI derivatives that are highly substituted to control this aggregation and then to incorporate them into devices. In addition, femtosecond transient absorption spectroscopy is being utilized to characterize these new active layer films. With this technique, we can monitor charge transfer to the PDI and optimize films for maximum charge separation.

POSTER 6: NOVEL SYNTHESIS OF NANOSTRUCTURED LaB6 POWDERS FOR HYDROGEN STORAGE APPLICATIONS

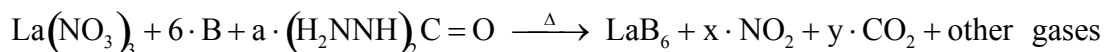
Raghunath Kanakala,^{*} Gabriel Rojas-George,⁺ and Olivia A. Graeve^{*}

^{*} Inamori School of Engineering, Alfred University, 2 Pine Street, Alfred, NY 14802, USA

⁺ Department of Chemical and Metallurgical Engineering

University of Nevada, Reno, 1664 N. Virginia Street – MS 388, Reno, NV 89557

The goal of this project was to demonstrate the feasibility of preparing nanocrystalline LaB6 powders via a controlled combustion synthesis process. These powders are extraordinarily strong electron emitters. When exposed to electric fields fast diffusion of the metal atoms is achieved. With a change in applied polarity hydrogen absorption and desorption can be achieved, thus serving as potential materials for hydrogen storage. The synthesis reaction for the preparation of the powders is described below.



During this process, controlled amounts of lanthanum nitrate (oxidizer) and amorphous boron were reacted with carbonylhydrazide (fuel) in a muffle furnace from room temperature to approximately 320°C. Some reactions made use of water for dissolving the reactants and some did not. As the reactants were heated, the oxidizer and fuel reacted to form a fine violet powder that contains both nanocrystalline LaB6 and unreacted boron. The presence of water during the reaction promoted the formation of some lanthanum borate, which is undesirable; thus, reactions without the use of water were more amenable for the formation of the LaB6. After synthesis, the unreacted boron and borate impurities were removed from the powders using a controlled HCl and H2SO4 wash. The resulting phase-pure and faceted LaB6 powders were then characterized using x-ray diffraction for phase purity and crystallite size, x-ray photoelectron spectroscopy for any free boron, scanning electron microscopy for particle morphology, and dynamic light scattering for particle size distribution. This project was funded by a grant from the US Army Research Office under contract number W911NF-06-1-0226 with Dr. William Mullins as project manager.

POSTER 7: DEVELOPMENT OF NEW SEMICONDUCTING POLYMERS FOR HIGH PERFORMANCE ORGANIC SOLAR CELLS

Yongye Liang and Luping Yu

Department of Chemistry and the James Franck Institute, The University of Chicago, 929 E. 57th Street, Chicago, IL 60637

Solar energy harvesting using the photovoltaic effect requires active semiconducting materials to convert light into electricity. Recently, solar cells based on organic materials showed interesting features, especially on the potential of low cost in materials and processing. Judging from the recent success in organic light emitting diodes based on the reverse photovoltaic effect, organic solar cells are very promising.¹ So far, after extensive optimization, power conversion efficiency of 4-5% has been achieved and confirmed in solar cells using regio-regular poly(3-hexylthiophene) (P3HT) as an electron-donor material and [6,6]-phenyl-C₆₁-butyric acid methyl ester (PC₆₁BM) as an acceptor material.² However, a bottleneck in conversion efficiency seems to be reached by using P3HT because it harvests photons with wavelength below about 650 nm, which is a small portion of the whole solar spectrum.³ Therefore, organic materials with low band gaps, which can efficiently harvest solar energy in broader spectrum, are needed in order to push these types of solar cells into practical application. The design of low band gap donor polymer materials requires judicious design.⁴ Most recently, low band gap polymer PV system showed over 4% efficiency with extensive device engineering efforts.⁵

Herein, a series of new low band gap polymers containing thieno-[3,4-b]thiophene unit have been developed for photovoltaic applications. Simple polymer solar cells based on PTB1 and methanofullerene [6,6]-phenyl-C₇₁-butyric acid methyl esters (PC₇₁BM) exhibit a solar conversion efficiency of 5.6%. An external quantum efficiency of 67% and fill-factor of 65% are achieved, both of which are among the highest values reported for a solar cell system based on a low bandgap polymer. This polymer system provides a solid foundation for further exploration in solar cells with real applications with future sophisticated material formulation and device engineering efforts.

1. Forrest, S. R. *Nature*, **2004**, 428, 911.
2. (a) Li, G.; Shrotriya, V.; Huang, J. S.; Yao, Y.; Moriarty, T.; Emery, K.; Yang, Y. *Nature Mater.* **2005**, 4, 864; (b) Ma, W. L.; Yang, C.Y.; Gong, X.; Lee, K. H.; Heeger, A. J. *Adv. Funct. Mater.* **2005**, 15, 1617.
3. Brabec, C. J. *Solar Energy Materials and Solar Cells* **2004**, 83, 273.
4. Roncali, J. *Macromol. Rapid Commun.* **2007**, 28, 1761.
5. (a) Peet, J.; Kim, J. Y.; Coates, N. E.; Ma, W. L.; Moses, D.; Heeger, A. J.; Bazan, G. C. *Nat. Mater.* **2007**, 6, 497. (b) Lee, J. K. ; Ma, W. L.; Brabec, C.J.; Yuen, J.; Moon, J. S. ; Kim, J. Y. ; Lee, K. ; Bazan, G. C. ; Heeger, A. J. *J. A. Chem. Soc.* **2008**, 130, 3619; (c)Wienk, M. M.; Turbiez, M.; Gilot, J.; Janssen, R. J. J. *Adv. Mater.* **2008**, 20, 2556.

**POSTER 8: BIOLOGICAL AND ENVIRONMENTAL TRANSFORMATIONS
ENGINEERED NANOPARTICLES AND IMPACTS ON DEVELOPMENTAL
TOXICITY**

Paige N Wiecinski¹, Kevin M Metz², Matthew J Bierman³, Song Jin³, Robert J Hamers³, Warren Heideman^{1,4}, Richard E Peterson^{1,4}, Joel A Pedersen^{1,2,5}

¹Molecular and Environmental Toxicology Center, ²Environmental Science and Technology Program, ³Department of Chemistry, ⁴School of Pharmacy and ⁵Department of Soil Science, Madison WI 53706

The unique properties of nanoscale materials that make them attractive from a materials science standpoint may also lead to undesirable biological outcomes. Few studies to date have examined the biological effects of engineered nanoparticles in whole organism systems (*in vivo*). Therefore understanding of the influence of nanomaterial properties on biological activity in intact animals is at an early stage. Biological modification and biogeochemical processing (i.e., weathering) of nanomaterials have the potential to alter their biological activity, but little is currently known about environmental or biological transformations of engineered nanomaterials and the biological effects of such modified nanomaterials. The toxicity of engineered nanomaterials is expected to be dependent not only on potential transformations in the environment, but also their persistence in biological systems. Because biogeochemical processing of engineered nanomaterials may alter their biological activity, we aim to elucidate the fundamental degradation chemistry of nanomaterials under representative biological and environmental conditions. Here, we demonstrate that exposures to simulated gastric fluids or oxidative environmental conditions degrade PEGylated CdSe_{core}/ZnS_{shell} quantum dots. Using the embryonic zebrafish assay, we show that oxidatively degraded quantum dots are more toxic than their intact counterparts and both exhibited higher toxicity than CdCl₂ alone. A fundamental understanding of the relationship between the structure of engineered nanoscale materials and adverse biological effects and those processes governing transformations of engineered nanomaterials in the environment and biological systems will facilitate the design of environmentally benign nanomaterials.

**POSTER 9: NANOMATERIAL EXPOSURES and BIOLOGICAL OXIDANT DAMAGE:
TOWARDS NEW EXPOSURE METRICS**

SHU-FENG HSIEH^{1,2}, EUGENE J. ROGERS¹, DANIEL SCHMIDT³, DHIMITER BELLO⁴

1-Department of Clinical Laboratory and Nutritional Sciences; 2-Multicampus Biomedical Engineering and Biotechnology Program; 3- Department of Department of Plastics Engineering; 4-Department of Work Environment; University of Massachusetts, Lowell, MA, USA

Industrial manufacturing and applications of engineered nanomaterials (NMs) are rapidly expanding. This development has brought with it potential for human exposure and environmental release, triggering a need for rapid screening of safety and health hazards of these materials. Toxicity associated with NM's as determined by complex in vitro and in vivo assays is associated with specific physicochemical characteristics, including specific surface area (SSA), transition metal content, surface charge, crystallinity, morphology, and agglomeration status. Complete characterization of these parameters requires substantial amounts of NM's, extensive expertise, time and modern facilities and can be done only with bulk materials. Additionally, NM exposures in the workplace and the environment do not allow for such extended characterizations.

Oxidative stress, widely implicated in the development of multiple diseases, has been suggested as a possible metric for evaluating toxicity potential of NMs. Our previous study validated the use of a Ferric Reducing Ability of Serum (FRAS) assay to determinate the oxidant damage of several NMs. The objectives of this research were to: i) explore underlying relationships between oxidative stress exerted by various NMs as determined by the FRAS and a comprehensive set of their physicochemical parameters; ii) to specifically test the hypothesis that FRAS may be used as a single complementary metric to screen for the bio-toxicity of bulk NM's.

The current work reports on the relationship between FRAS and several key parameters: specific surface area (SSA) as determined by the N₂ adsorption BET technique; transition metal content determined by instrumental neutron activation analysis; crystallinity determined by X-ray diffraction; surface charge determined with a ZetaPals instrument in PBS saline and soluble transition metals content by inductively coupled plasma –mass spectrometry (ICP-MS). SSA was generally, but not always, significantly associated with the degree of oxidative stress and so was the presence of select transition metals, especially Fe, Cr, Co, and Mo. This partial analysis reveals complex and often difficult to predict relationships between oxidative stress and NM properties and provides credibility to the utility of FRAS as a better metric for toxicity screening and possibly for characterization of airborne exposures. Work-in progress is investigating the influence of crystallinity, surface charge, and extractable metals on these relationships and is developing a modified FRAS method for airborne NM exposures.

POSTER 10: MODELING THE RESISTANCE AND FILL FACTOR LIMITS IN BULK HETEROJUNCTION ORGANIC PHOTOVOLTAICS

Jonathan D. Servaites, Mark A. Ratner,* Tobin J. Marks*
Department of Materials Science and Engineering,
Northwestern University, Evanston, IL USA

Organic photovoltaics (OPVs) offer the potential for lowering the cost of solar energy. However, we must first overcome significant scientific and technical hurdles, including low conversion efficiencies. State of the art OPV cells use the so-called bulk heterojunction (BHJ) architecture, which incorporates a blend of the donor and acceptor organic semiconductors, instead of using a bilayer structure. Given this design and the unique attributes of the materials used in these cells, there exists the need to develop modeling approaches for these devices. We address this problem, first, by showing that BHJ OPVs can be effectively modeled through a numerical diode-based model. This method is useful in articulating the limits of ideal behavior and the benefits of improving the cells' ohmic and shunt losses and diode factor. Our analysis shows that state of the art OPVs are already approaching ideal behavior for the fill factor and resistance parameters. Ultimately, these results demonstrate that OPV materials research should focus on other metrics, such as absorption characteristics and the open circuit voltage, to further improve device conversion efficiencies.

POSTER 11: REAL-TIME MEASUREMENTS DURING ELECTROSPINNING OF POLYSTYRENE USING RAMAN SPECTROSCOPY

G.Gururajan, C.Giller, C.Snively, D.B.Chase and J.F.Rabolt*
Department of Materials Science and Engineering, University of Delaware, Newark, DE- 19716.

Electrospinning is an important technique to make polymeric nanofibers. As in any polymer processing technique, the history of fiber formation influences its microstructure, which in turn determines the properties. Therefore, real-time measurements during electrospinning can help in a better understanding of the process through formulation of process-structure-property correlations. Real-time Raman spectroscopy was attempted to monitor the solvent evaporation during electrospinning of atactic polystyrene (a-PS). The importance of jet stability for real-time measurements has been reported in a previous study. Therefore, a binary solvent system of N, N-dimethyl formamide (DMF) and tetrahydrofuran (THF) with a-PS was used in this study which insured a stable straight jet during the experiment. The strong Raman bands at 866 cm^{-1} , 914 cm^{-1} and 1004 cm^{-1} unique to DMF, THF and a-PS respectively, were used to evaluate concentration profiles for different processing parameters.

* Corresponding author: rabolt@udel.edu

Appendix 4: Research Abstracts and Biographical Information for Chinese Delegates

Prof. Zhanguo Wang (王占国)

Wang Zhanguo [Z. G. Wang] was born on Dec. 29 of 1938 in Henan province, China. He graduated from the Department of Physics, Nankai University, China in 1962. Then he immediately joined the Institute of Semiconductors, Chinese Academy of Sciences (IS, CAS), engaged in studies on semiconductor materials physics and materials characterization till 1980. From 1980 to 1983, he was a visiting scientist at the Department of Solid State Physics, the University of Lund, Sweden, working on spectrum physics and deep levels physics of semiconductors. By the end of 1983 he came back to China, and became a research professor and a head of Semiconductor Materials Division of IS, CAS in 1986. From 1990, Prof. Wang served as director of Key Lab. of Semiconductor Materials Science and a deputy director of the IS, CAS, the member of National Advanced Materials Committee of China (NAMC), vice president of Chinese Materials Research Society and director of Semiconductor and Integration Technology Society, the Chinese Institute of Electronics etc. Prof. Wang was elected as a member of the CAS in 1995. From 1994 till now, his research work has concentrated to semiconductor nanostructures growth and related quantum devices fabrication. He has published 3 books and more than 180 refereed papers in many authoritative journals since 1983. And he was awarded a number of prizes from the Nation and from the Chinese Academy of Sciences.

RDS Characterization of wetting layer around InAs/GaAs Quantum Dots by SK Growth Mode

Zhanguo Wang (王占国)

Key Lab. Of Semiconductor Materials Science Institute of Semiconductors,
Chinese Academy of Sciences, P. O. Box 912, Beijing 100083, China

zgwang@semi.ac.cn

Self-assembled quantum dots (QDs) formed by Stranski–Krastanow (SK) growth have attracted much attention due to their potential application in novel devices. However, the optical and electrical properties of the self-assembled QDs can be greatly affected by wetting layer (WL) around the dots, because the WL can behave as channels for carriers to escape from and redistribute among the dots, strongly influencing the temperature dependence of the emission wavelength. The modulation response of QD lasers could also be limited by WLs. Therefore information about the electronic states and structures of WLs is desirable for a complete understanding of the behavior of QDs and their devices. However, it is quite difficult to access information experimentally about WLs. In this letter, reflectance difference spectroscopy (RDS) will be adopted to characterize the WL in the InAs/GaAs system. RDS is a sensitive tool for characterizing the in plane optical anisotropy (OA) of surfaces and quantum wells, in which the symmetries are reduced due to the surface reconstruction and the inversion asymmetry of the quantum wells, respectively. The OA is also expected for WL, which behaves actually as an asymmetric QW due to the segregation effect of indium. One transition related to the light hole in the WL has been observed clearly in Reflectance difference spectroscopy (RDS), from which its transition energy and in-plane OA are determined. The evolution of WL with the InAs dot formation and ripening has been discussed.

Prof. Yong Cao (曹 镛)

Yong Cao was born in Changsha, China. He received his Bachelor Degree in Chemistry in former Leningrad University (Russia) at 1965. Then at 1966, he joined Institute of Chemistry, Chinese Academy of Sciences (ICCAS), Beijing, and he has been appointed as full Professor of ICCAS since 1986. In 1979-1981 he was visiting scientist in Department of Chemistry (Prof. H. Kuroda Lab of Physical Chemistry 2), Tokyo University (Japan) where he received his PhD degree in physical chemistry in 1987. In 1988-1990 he was visiting researcher in Institute of Polymer and Organic Solids, University of California, Santa Barbara (Prof. Alan Heeger's group). In 1990 he joined UNIAX Corporation founded by Alan Heeger and Paul Smith. In 1995, he became UNIAX Fellow (lately, DuPont Displays Fellow after acquisition of UNIAX corporation by E. I. du Pont de Nemours & Company, Inc.) Since 1998, he has been appointed as full professor, director of Institute of Polymer Optoelectronic Materials and Devices, South China University of Technology, Guangzhou, China. He is member of Chinese Chemical Society, American Chemical Society and SPIE.

His fields of research include conducting polymers, optoelectronic conjugated polymers and devices (electroluminescent and photovoltaic devices). Yong Cao is co-author of approximately 400 scientific papers and co-inventor of more than 20 US patents in the areas of conducting polymers and optoelectronic polymers devices.

Studies and recent Progress of Polymer Bulk-Heterojunction Photovoltaic Devices

Yong Cao, Institute of Polymer Optoelectronic materials and Devices,
South China University of Technology, Guangzhou, 510640, P.R.China

Abstract: Photovoltaic devices by using organic and polymer materials have been attracted considerable interest recent years. Among varieties of concepts proposed for organic/polymer solar cells, the polymer bulk heterojunction solar cell is one of the most attractive and promising approaches. After brief introduction of mechanism of polymer heterojunction solar cells and recent progress worldwide and in the Mainland of China, we will concentrated on recent studies and progress performed at SCUT group. This will include our research in the following aspects:

1. Synthesis and device performance of new donor and acceptor materials
2. Nanomaterials synthesis for polymer/inorganic semiconductor hybrid photovoltaic devices
3. Morphology control and interface optimization
4. Efforts towards to all-printable optoelectronic device

The limiting factors for such type of devices and future perspective for solution processable, large area polymer solar cell will be discussed.

Prof. Jian Xu (徐 坚)

Jian Xu, PhD was born on Jun. 29, 1961 in Helongjiang Province, P. R. China. He is Professor of Institute of Chemistry, Chinese Academy of Sciences (ICCAS), Pluralistic Professor of Peking University, Sichuan University, Wuhan University. He earned his Ph.D. in 1994 from Sichuan University, China, his M.S. degree in 1985 and his B.S. in 1982 from Chengdu University of Science and Technology. He served as lecturer at Beijing Institute of Chemical Technology from 1985-1992, a Postdoctoral fellow at Institute of Chemistry, Chinese Academy of Sciences (ICCAS) from 1995-1996 and a Visiting Scientist, at the University of Hokkaido, Japan from 1998-1999. His current research interests focus on the architecture of bionic microstructure and morphology of polymer and its unconventional properties, condensed dynamics and smart behaviors of bionic polymer, advanced materials of functional polymer and optical polymer fiber, etc. Since 1985, he has published about 140 papers, 23 patents were authorized, 22 patents were applying, 7 Academic Books and 6 chapters were published. Prof. Xu also serves as the Vice Director of the Chinese Materials Research Society (C-MRS).

Facile Creation of Biomimetic Systems at Interface

Jian Xu*, Xiaoyan Zhang, Ning Zhao, Xiaoying Lu, Qiongdan Xie, Lian Zhang and Xiaoli Zhang (State Key Laboratory of Polymer Physics and Chemistry and National Laboratory of Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences (ICCAS), Beijing 100190, (P. R. China))

Abstract: Nature always gives us inspirations for fabricating functional materials by mimicking the structure design of biomaterials. Functional surfaces with special wettabilities like superhydrophobicity and superamphiphobicity have attracted lots of research interests because of their great advantages in applications, such as self-cleaning effect, anti-adhesion, anti-erosion, current-conduction inhibition, *etc.* However, the strict preparation conditions, multi-step processes and high cost of the methods to create biomimetic interface, limited their practical applications. Therefore, developing simple, cheap but effective method becomes the focus of our research in this field. In this report, facile methods for creating lotus-leaf-like micro-nano-binary structured superhydrophobic or superamphiphobic surfaces based on different mechanisms, *i.e.*, solvent induced phase separation of blend polymer solution, self-assemble of copolymer micelle solution, solvent induced crystallization, were developed. Moreover, some progresses in investigation on the special microstructure induced unique wetting properties were also introduced.

Keywords: biomimetic systems, surface, superhydrophobicity, wetting behavior, microstructure

Prof. Yunqi Liu (刘云圻)

Liu Yunqi, PhD was born on February 22, 1949 in Jiangsu Province, PR China. He is currently Professor of Chemistry at Institute of Chemistry, Chinese Academy of Sciences. His educational and professional appointments include: 1972.04–1975.07, Department of Chemistry, Nanjing University; 1975.08–present, Institute of Chemistry, Chinese Academy of Sciences, among which: 1985.01–1988.03, a PhD student in the Institute of Physical and Chemical Research, Japan; 1991.04–1991.10, preparation for PhD defense in Tokyo Institute of Technology (TIT), Japan, and received Dr. degree from TIT, Japan; 1997.10–1998.08, a visiting scholar in Northeastern University, USA; 2000.03–2000.06, a visit professor in The Ohio State University and in University of Washington, USA 2003.04–present, part-time professor, Department of Chemistry, Tsinghua University; 2004.01–2004.04, guest professor, Kyoto University; 2008.01–present, part-time professor, Department of Chemistry, Wuhan University. His current research interests include design and synthesis of molecular materials, organic/polymeric light-emitting diodes, organic field-effect transistors, and preparation of carbon nanotubes and their electronic devices. His awards include the 2007 National Natural Science Award (2nd).

Design and Synthesis of High Mobility Materials and their Application in Organic Field-effect Transistors

Yunqi Liu

(Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China)

Organic field-effect transistors (OFETs) have attracted much attention due to their potential applications in low cost, large-area, and flexible electronic devices. Great progress has been achieved so far in the organic FETs, whose mobilities are comparable to those of amorphous silicon FETs.

The organic semiconductors play a key role in determining the device characteristics. The properties of the organic semiconductors such as molecular structure and packing as well as molecular energy levels can be properly controlled by molecular design. Therefore, we designed and synthesized a series of organic molecules. The synthesized organic semiconductors exhibit excellent field-effect properties due to strong intermolecular interactions and proper molecular energy levels. Meanwhile, the influence of the device fabrication process, organic semiconductor/dielectric layer interface, and organic layer/electrode contact on the device performance was investigated. Furthermore, single crystal field-effect transistors were fabricated because the single crystal based FETs can provide accurate conducting mechanism of organic semiconductors and higher device performance compared with those of the thin film FETs.

In this presentation, a series of novel organic molecules designed and synthesized in my research group and their application in field-effect transistors are introduced.

Keywords: Organic semiconductors, Field-effect transistors, High mobility

Prof. Qingbo Meng (孟庆波)

Qingbo Meng, PhD, was born on Oct. 07, 1964 in Jilin Province, PR China. He is a Professor at the Institute of Physics, Chinese Academy of Sciences, Beijing China. He earned his Ph.D. in 1997 from the Changchun Institute of Applied Chemistry (CIAC), Chinese Academy of Sciences and his B.Sc. degree in 1987 at the Department of Physics, Jilin University in Changchun, China.

His appointments include: Postdoctoral Fellowship from 1997 to 1999 at Institute of Physics, CAS, China; STA Fellowship at the Science and Technology Agency of Japan and Researcher of KAST of Japan and the University of Tokyo from 1999 to 2002. In 2001, he was selected as a member of "Hundreds of Talents" of CAS. In 2002, he worked for a short time as a NEDO Fellow of Research Institute of Innovative Technology for the Earth (Japan).

Since 2001, His research has focused on solar materials and devices, *i. e.* dye-sensitized solar cells; the design of photocatalysts for photosplitting water and photodegradation; photonic crystal self-assembly. Up to now, more than 60 scientific papers have been published and 18 patents have been applied (4 patents authorized) for scientific exchange.

He is a member of the Chinese Renewable Energy Society and currently serves as its Vice Director. He is also a member of Chinese Physics Society and Chinese Chemistry Society, Editor Board of Electrochemical Communications, Deputy Director of Clear Energy Center, and the Institute of Physics, Chinese Academy of Sciences.

Prof. Hui-Ming Cheng (成会明)

Hui-Ming Cheng is a Professor and Executive Deputy Director of the Institute of Metal Research, Chinese Academy of Sciences. He also heads the Advanced Carbons Division of Shenyang National Laboratory for Materials Science. He worked at Kyushu National Industrial Research Institute from 1990 to 1992 and Nagasaki University from 1992 to 1993 in Japan, MIT in USA from 1997 to 1998, and at Nanyang University of Technology in Singapore, University of Queensland in Australia since 2000. He has received major research funds from National Science Foundation of China, Ministry of Science and Technology of China, Chinese Academy of Sciences, some funding agencies in other countries, and several global corporations. He leads several national key projects in nanomaterials, nanotechnology and new energy fields, particularly the synthesis and applications of carbon nanotubes and energy storage materials.

He has published a book entitled Carbon Nanotubes: Synthesis, Structure, Properties and Applications in Chinese, several book chapters, and authored or co-authored over 220 peer-reviewed English papers published in Science, Nature, Adv Mater, NanoLett, Adv Func Mater, Angewandte Chemie Inter. Ed. Chem of Mater, Carbon, ACS Nano, APL, etc. which have been cited more than 3100 times. He has received several awards, including National Natural Science Award (2nd class) in 2006, China Science and Technology Award for Young Scientists in 2000, and the Khwarizmi International Award in 2007. He serves on several expert panels, and as Editor of Carbon since 2000 and Editor-in-Chief of New Carbon Materials since 1998.

His research activities now mainly focus on the synthesis, properties, and applications of carbon nanotubes, graphenes, new energy materials, and advanced carbon materials. In particular, he is working on novel materials for lithium ion batteries and supercapacitors, hydrogen storage materials with high capacity, and novel photochemically active materials for high-efficiency solar energy conversion in recent years, in order to lead scientific understanding and technological innovations in sustainable development of energy and environment.

Prof. Feiyu Kang (康飞宇)

Feiyu Kang, was born on Sep. 21, 1962 in Nei Mongol, PR China. He is Professor of Materials Science and Engineering at Tsinghua University in Beijing, China. He obtained a Ph.D. degree in Mechanical Engineering from the Hong Kong University of Science and Technology in 1997. He earned a Masters in Mechanical Engineering in 1988, and a B.Sc. degree in Mechanical Engineering in 1986, both from Tsinghua University. He was a Research Associate at Hokaido University, Japan from Sep. to Dec. 1997.

Prof. Kang's research interests include graphite process; graphite intercalation compounds; lithium ion battery; EDLC; fuel cell; porous carbon and adsorption, etc. He has published one book and more than 100 scientific papers.

On the social activities, Prof. Kang is currently a Provost of Tsinghua University, Associate Editor in Chief of Journal of New Carbon Materials, Advisory Board member of Journal of Carbon; International Advisory Board member of International Symposium on Intercalation Compounds.

Prof. Yichun Liu (刘益春)

Yichun Liu, PhD was born on Dec. 29, 1962 in Jilin Province, PR China. He is Professor of Physics at Center for Advanced Optoelectronic Functional Materials Research, School of Physics, Northeast Normal University, Changchun, China. In 1995, he obtained a joint PhD from Changchun Institute of Physics, Chinese Academy of Sciences (CAS) and Polytechnic of Turin, Italy. He obtained his MSc. Degree in 1988 at the Changchun Institute of Physics and his B.Sc. in 1985 at the Department of Physics, Northeast Normal University in Changchun. He was a post doctoral fellow in Chemistry at Jilin University from 1996-1998, and a visiting professor at Kyushu University in Japan from 1996-1997. Since 1996, his research has concentrated on wide gap-band semiconductor materials, in particular, on the growth of nano-ZnO and ZnO films, heterojunction device etc. He has published more than 120 scientific papers and been cited over 1000 times. Professional achievements include National science foundation for distinguished young scholars (2007), Excellent fellow of Hundred Talents, Chinese Academy of Sciences (2003), and 1st prize for natural science by the ministry of education (2006).

His society memberships include: Vice-chairman of physical society of Jilin province, Chairman of physical society of Changchun city; Deputy Editor of Chin. J. Luminescence and Deputy Editor of Chin. J. Phys. Expt.

His representative publications include:

1. Chen S J, Liu Y C*, Shao C L, et al., "structural and optical properties of uniform ZnO nanosheets", **Adv. Mater.** 17 (2005) 586.
2. Ma J G, Liu Y C*, Shao C L, et al., "Formation and luminescence of ZnO nanoparticles embedded in MgO films", **Phys. Rev. B** 71 (2005) 125430.
3. Chen S J, Liu Y C*, Shao C L, et al., "Photoluminescence study of ZnO nanotubes under hydrostatic pressure", **Appl. Phys. Lett.** 88 (2006) 133127.
4. Li XH, Shao CL, Liu YC*, "A simple method for controllable preparation of polymer nanotubes via a single capillary electrospinning", **LANGMUIR** 23(2007)10920
5. Liu YC*, Zhong MY, Shan GY, et al., "Biocompatible ZnO/Au nanocomposites for ultrasensitive DNA detection using resonance Raman scattering", **J. Phys. Chem. B** 112 (2008) 6484.
6. Xiao ZY, Liu YC*, Mu R, et al., "Stability of p-type conductivity in nitrogen-doped ZnO thin film", **Appl. Phys. Lett.** 92 (2008) 052106

Prof. Jiaguo Yu (余家国)

Jiaguo Yu, PhD was born on Jan. 29, 1963 in Hubei Province, PR China. He is Professor of Materials Physics and Chemistry at State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan 430070, China. He obtained his Ph.D. in 2000 at the State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, China. He earned his MSc. In 1988 at the School of Chemical Engineering, Xi'an Jiaotong University, Xi'an, China and his B.Sc. in 1985 from the Department of Chemistry, Huazhong Normal University, Wuhan, China. He was a Postdoctoral Fellow from Nov. 2000 to May 2002 and July 2003 to July 2004 at The Chinese University of Hong Kong. He was a Visiting Scientist from Nov. 2005 to Oct. 2006 at the University of Bristol (Prof. S. Mann's group), in Bristol, UK and Visiting Scholar from Oct. 2007 to April 2008 at University of Texas at Austin (Prof. Allen J. Bard's group), Austin, USA.

Since 2000, his research is concentrated on semiconductor photocatalytic materials and their environmental application (such as water and air purification), nanoporous and hollow materials, nanomaterials and nano-structured materials, biomimetic synthesis, biocrystallization and morphology control, etc.

He has published more than 150 scientific papers for scientific exchange. On the social activities, he is a member of the Editorial Board of Journal of Hazardous Materials.

Prof. Duan Weng

Duan Weng was born on Nov. 01, 1957 in Anhui Province, PR China. He is Professor of Ecomaterials at Department of Materials Science and Engineering, Tsinghua University, Beijing 100084, China. He earned his Ph.D. in 1995 at the Department of Materials Engineering, Swiss Federal Institute of Technology Zurich (ETH), Switzerland, his MSc. Degree in 1985 at the School of Chemical Engineering, Dalian University of Technology, Dalian, China, and his B.Sc. in 1982 at the Department of Chemical Engineering, Dalian Institute of Technology, Dalian, China.

He was a Visiting Professor from Sep. 2002 to July 2003 at Yale University, New Haven, USA, and the Visiting Professor from September 2004 to March 2005 at University of Washington, Seattle, USA.

Since 1996, his research interests have focused on ecomaterials, eco-design, resource reproductivity, recycling, environmental impact of materials, etc. He has published 7 books and more than 120 scientific papers. He is currently the Deputy Secretary General and Executive member of Chinese Materials Research Society (C-MRS).

Appendix 5: Working Group Guidelines

The purpose of the working group sessions is to:

1. Generate recommendations for improving US-China collaborations in areas of common interest and complementary strength.
2. Discuss and plan potential joint projects for addressing energy and environmental challenges.

Each working group is asked to develop a brief report (in PowerPoint and Word format) answering the following questions:

Part 1: Recommendations for improving US-China collaborations

- What are some barriers to US-China collaboration?
- How can these barriers be overcome (i.e., what mechanisms / joint programs/ strategies - new and existing)?
- What are some important complementary strengths in the US and China (i.e., research capabilities, know-how, infrastructure, education capabilities, etc.)
- What are your suggestions for improving networking?

Part 2: Some potential joint research projects in energy and environment

- Project Title (s)
- Rationale
- Goals
- Required expertise and potential participating institutions in US and China
- Collaboration structure (center, institute, university network, etc.- how will it function?)
- Complementary facilities and capabilities
- Anticipated outcomes
- Broader impact, including integration of research with education
- Budget considerations
- Action items

Part 3: “Big-picture” recommendations for enhancing US-China cooperation in these areas?

Appendix 6: Working Group Reports

Working Group 1: Advanced Solar Cell - A

Bruce Parkinson, University of Wyoming (US) – *Co-leader*

Zhanguo Wang, Institute of Semiconductors, CAS (China) – *Co-leader*

Geoffrey Hutchison, University of Pittsburgh (US) – *Scribe*

Luping Yu, University of Chicago (US)

Tobin Marks, Northwestern University (US)

Ethan Good, Dow Corning Corporation (US)

Qingbo Meng, Institute of Physics, CAS (China)

Yongye Liang, University of Chicago (US) - *Student*

Charusheela Ramanan, Northwestern University (US) - *Student*

Bilal El-Zahab, Louisiana State University (US) - *Postdoc*

1. Recommendations

Near-term:

- Improved transportation of scientific equipment and samples between the US and China is critical for continued collaboration.
- Continued improvement on obtaining US visas for Chinese students and scientists is critical. Recent efforts from the NSF, including an office in Beijing are greatly appreciated and should be encouraged to expand. Support letters from NSF program officers and others do speed visa requests, but some are still denied or delayed inexplicably.
- Improved cyberinfrastructure to facilitate networking, including open databases of research expertise, unique complementary facilities and equipment, and materials properties.
- Networking can be facilitated by encouraging undergraduate, graduate student, postdoctoral, and senior personnel exchange programs on both sides. Such visits should include significant time, including student summer research exchanges, and funding for 1-2 week visits for mini-courses and lecture series for both US scientists in China and Chinese visitors to the US.
- Bilateral networking and social activities should be encouraged at major scientific conferences as satellite meetings. These interactions can be slightly before or after large conferences to leverage attendance and minimize cost, travel and time requirements.

Long-term:

- Such near-term efforts should be continued in the long-term, particularly under the aegis of a global effort to address fundamental challenges in solar materials, including both advanced photovoltaic electrical generation and energy storage including solar fuel generation and improved battery and supercapacitor devices.
- Challenges in advanced solar materials require addressing fundamental scientific and technological grand challenges across disciplines and national boundaries. These include: Understanding all appropriate interfacial effects on optoelectronic organic and inorganic materials; Characterizing and understanding all loss mechanisms (electrical, optical, etc.) at contacts and donor/acceptor interfaces; Rational design and optimization of novel organic and inorganic materials and nanoarchitectures with an aim for improved, highly efficient photovoltaic devices; Development of advanced characterization techniques for addressing

and understanding buried nanoscale interfaces; Developing predictive theoretical / computational models of nanoscale and mesoscale optical effects, charge transport, and material structure, particularly in realistic interfaces and defects.

2. The Big Picture

- a. US-China leadership in global energy and environmental challenges
- b. Vision and mission (e.g., the establishment of a Global Energy Institute)

3. Potential research projects

We derived three potential collaborative research projects: (1) “Understanding and Controlling Organic Phase Segregation in Bulk Heterojunction Photovoltaic Materials”; (2) “Overcoming Charge Transport Limitations in Organic Bulk-Heterojunction Photovoltaics”; and (3) “Nanostructured Inorganic/Organic Hybrid Photovoltaic Devices”, which are described below

Project 1: “Understanding and controlling organic phase segregation in bulk heterojunction photovoltaic materials”

Rationale: A critical issue with organic bulk heterojunction devices is the morphology and inherent charge-transport percolation network. This directly controls the separation of created excitons and the mobility of generated photocarriers.

Goals: (1) Understanding the issues which affect morphology and phase separation at the nanoscale requires advanced characterization techniques; (2) Understanding how surface area and phase segregation affect carrier generation and loss mechanisms; (3) Developing predictive theoretical / computational models of nanoscale and mesoscale phase evolution; (4) Use this information to design synthetic modifications to donor and acceptor components with desired morphologies.

Required expertise and potential participating institutions (US and China): Polymer theory; Multiscale computational modeling; Nanostructural physical and photophysical characterization; Charge transport characterization over broad timescale (i.e., DC, AC, long-term stability); Synthesis and processing

Collaboration structures (center, institute, university network – how will it function)

- Complementary research groups at centers, institutes and universities:
- Personnel exchange
- Sample exchange
- Joint measurement (to ensure consistent correlation)
- Iterative process of model improvement (synthesis, characterization, theory)

Anticipated outcomes

- Increased control of morphology at the nanoscale.
- Improved modeling capabilities (theory, software, and cyberinfrastructure with improved functionality)
- Greatly enhanced power conversion efficiencies in large-area bulk heterojunction devices.

Broader impact, including integration of research with education

- Less expensive, more efficient bulk heterojunction organic photovoltaic devices for large-scale deployment.
- Technical workforce capable of working in this emerging research area of organic optoelectronic materials
- Educated workforce capable of international collaborations and cultural exchange

Project 2: “Overcoming Charge Transport Limitations in Organic Bulk-Heterojunction Photovoltaics”

Rationale: The efficiency of a photovoltaic device is limited to the conversion of photons into charge carriers and extracting them. Existing devices exhibit low efficiencies.

Goals: (1) Demonstrate, understand and control singlet exciton fission and multi-exciton generation; (2) Understand and control 2D charge transport; (3) Characterize and understand all loss mechanisms (electrical, optical, etc.) at contacts and donor/acceptor interfaces; (4) Use this information to rationally design novel device architectures with improved efficiencies.

Required expertise and potential participating institutions (US and China): Spectroscopy over broad timescale (fast characterization of photogenerated carriers); Charge transport modeling including treatment of defects and interface interaction; Characterization of buried interfaces; Nanostructural physical and photophysical characterization; Charge transport characterization over broad timescale (i.e., DC, AC, long-term stability); Synthesis and processing

Collaboration structures (center, institute, university network – how will it function)

- Complementary research groups at centers, institutes and universities:
- Personnel exchange
- Sample exchange
- Joint measurement (to ensure consistent correlation)
- Iterative process of model improvement (synthesis, characterization, theory)

Anticipated outcomes

- Increased control of interfacial effects on charge transport and exciton recombination at the nanoscale.
- Improved modeling capabilities (theory, software, and cyberinfrastructure with improved functionality)
- Greatly enhanced power conversion efficiencies in large-area bulk heterojunction devices.

Broader impact, including integration of research with education

- Less expensive, more efficient bulk heterojunction organic photovoltaic devices for large-scale deployment.
- Technical workforce capable of working in this emerging research area of organic optoelectronic materials
- Educated workforce capable of international collaborations and cultural exchange

Project 3: “Nanostructured Inorganic/Organic Hybrid Photovoltaic Devices”

Rationale: The efficiency of a photovoltaic device is limited to the conversion of absorbed photons into electrons. Photons outside the semiconductor band gap are not currently utilized.

Goals: (1) Integrating organic photovoltaic materials into nanostructured inorganic devices; (2) Pairing of optimal organic photovoltaic materials and appropriate nanostructured inorganic semiconductor; (3) Introduction of surface functionalization at organic/inorganic interface to control wetting, charge blocking, adhesion/cohesion, and manipulate surface dipoles and charge injection; (4) Use of nanostructured inorganic material to control organic morphology and microscopic and long-range order.

Required expertise and potential participating institutions (US and China): Organic synthesis and processing; Inorganic synthesis and surface preparation; Characterization of buried interfaces, including spectroscopy, AFM, TEM, FT-IR, Sum-Frequency Generation; Charge transport modeling including treatment of defects and interface interaction; Theory of adsorbed organic molecules on nanostructured inorganic surfaces; Charge transport characterization over broad timescale (i.e., DC, AC, long-term stability)

Collaboration structures (center, institute, university network – how will it function)- See above. Required expertise maps into separate, complementary components

Complementary facilities and capabilities

Complementary research groups at centers, institutes and universities:

Personnel exchange

Sample exchange

Joint measurement (to ensure consistent correlation)

Iterative process of model improvement (synthesis, characterization, theory)

Anticipated outcomes

- Increased control of organic/inorganic interfacial effects on charge transport and exciton recombination at the nanoscale.
- Demonstration of improved photon capture due to synergistic organic and inorganic materials design.
- Improved modeling capabilities (theory, software, and cyberinfrastructure with improved functionality)
- Greatly enhanced power conversion efficiencies in large-area bulk heterojunction devices.

Broader impact, including integration of research with education

- Less expensive, more efficient photovoltaic devices for large-scale deployment.
- Technical workforce capable of working in this emerging research area of both organic and inorganic optoelectronic devices.
- Educated workforce capable of international collaborations and cultural exchange

Working Group 2: Advanced Solar Cells - B

Micheal Wasielewski, Northwestern University (US) – *Co-leader*

Yong Cao, South China University of Science & Technology (China) – *Co-leader*

Stefan Bernhard, Princeton University (US) - *Scribe*

Yang Yang, University of California at Los Angeles (US)

Thuc-Quyen Nguyen, University of California at Santa Barbara (US)

Bruce Parkinson, Colorado State University (US)

Yunqi Liu, Institute of Chemistry, Chinese Academy of Science (China)

Meng Guo, University of Michigan - *Student*

Jon Servaites, Northwestern University - *Student*

Shannon Riha, Colorado State University - *Student*

Complementary Strengths: China: materials synthesis; Strong math skills; Highly motivated workforce US: student training; More collaborative environment; Peer-review system for proposals and publications is better developed; IP protection and development.

Barriers / Challenges to US-China Cooperation: The following are barriers to cooperation: unfamiliarity with each other's research, which is even more emphasized by the distance and language barriers. This is played out in the different research and student mentoring styles. Also relevant are immigration issues and materials exchange across borders, not only with the initial start up, but also as the collaborations continue. Further down the road, the significance of the intellectual property questions could arise and cause complications.

Overcoming Barriers: Some possible avenues to overcome such barriers between the US and China need to be developed. Examples of overcoming the unfamiliarity with each other's research would be to construct expertise and skill databases for each respective country, as well as a materials structure and property database. To overcome the distance barrier, setting up remote tutoring labs and remote instruction, such as iLabs, which is currently being implemented at Northwestern and MIT through NSF, is suggested. To promote social interactions and address cultural differences between each country, involving students in exchange programs is crucial. Such programs would include: research group to research group visits, summer programs for undergraduates (REU program) and first-year graduate students, as well joint meetings. These different programs would facilitate discussion on emerging areas of research as well as familiarize each individual with other approaches to solve pressing global problems. Collaborations in such an area have to start from the bottom up and seed funding is crucial to augment such a collaborative climate. Starting with simple proposals with timely evaluation mechanisms would allow for effective initiation and continuation of the nascent collaboration. Since the students fuel and drive the collaboration, funding for travel grants for them would permit efficient exchange of ideas and expertise.

Recommendations:

1. Workshops in US and China in the area of Global Energy with the following components:
 - For the guest country participation by at least as many students as faculty
 - Tutorial overviews by invited speakers, not to include the speakers results but outlining the current-state-of-the-art and future challenges
 - Student poster sessions

- Matching of each guest student with a host student
- Laboratory visits
- Student run breakout sessions
- Cultural events
- Topical themes limited to a specific sub-area of research or could be broad in extent of coverage. Participation limited to 60 with a minimum of 40% being from the guest country.

2. IRCEU Sites-International Research and Cultural Experience for Undergraduates.

- This would be a 10 week program in which student from the US-visit Chinese Laboratories and vice versa. Each country covers travel costs, each host institution cover housing costs.
- Program is for 10 students and 10 mentors per site
- In US language is exclusively English; in China US student receive some formal introduction to Chinese for ~1 hour/day; English language speaking class is available
- Students receive training common to other REU programs including writing of proposal, research summary, how to keep notebook, responsible conduct in research, graduate opportunities.
- Institutions with strong record for successful REU site strongly encouraged to apply
- Each student houses with student from guest country; Cultural Activities included.

3. NSF-US-China International Graduate Fellowship

- This is a one or two year fellowship program in which 50% of the time is spent abroad. The program pays \$35,000/yr and includes travel costs and an allowance for foreign language training. Students from China are expected to be fluent in English and US students will be expected to complete one semester of Mandarin or equivalent, prior to their departure.
- The proposal will include the following components: Statement of purpose; statement of thesis outline and research completed to date; detailed research proposal describing the research to be performed in the host country and why this could be more effectively performed in a collaborative environment; letter of invitation outlining the willingness of the host institution to accept the student and provide assistance with all aspects of the students stay; letter of endorsement from the students advisor; two letters of recommendation.
- International exchange fellows will be expected to have periodic email or telephone exchanges with their stateside advisors during the course of the visit. They also will be encouraged to keep a journal to record their experiences, activities, and thoughts during the visit. The journal will provide a place where students may reflect on the new insights they are gaining not only concerning their projects, new research ideas, and collaborators but also about cross-cultural communication, scientific collaboration, their career paths, and the effects of this experience on their professional development. The journal activity is expected to assist students as a resource document as they prepare their final reports.
- Within a month of their return to the host country students will submit to the advisor a post-visit technical report describing project outcomes and the new knowledge acquired. Students will also be asked to include a short qualitative statement describing the perspectives gained on cultural aspects of science, technology, and research and how this experience has enhanced their professional development.

- **Evaluation Plan:** The student advisor will work with students to conduct a pre-travel and post-travel assessment of the students' technical skills. The pre-travel phase will involve an assessment of the student research plan and goals for the visit, logistical plan, and language/cultural preparation. Furthermore, the students advisor will in collaboration with the student submit a final report on outcomes, including how these international experiences have enriched students' professional lives, outlining the research accomplishments of the international fellows, and describing how the program has furthered the goals of the research to strengthen research ties with the international partners. The student's advisor will solicit input from the international partners about the success of the experience.
- **Benefits of the International Exchange Program:** There is a clear need for US and Chinese students to understand and be able to compete in a global market and this requires developing ties with international collaborators early in their careers, and requires students to understand that they can successfully integrate in a culture very different from what they experience in their day to day life in the US and China. In the past a program to foster such goals would have been viewed as a luxury, but in the current climate of outsourcing and globalization of economy, international training will become an essential component of the education experience of our next generation of leaders, thus this program fits extremely well into NSF's and NSFC's long term strategy of mentoring its students to become the next generation of leaders in both academic, industrial and government environments.
- We have emphasized that these exchanges be considered an integral part of the graduate education process and therefore they should not unduly prolong the graduation process for participants. With this understanding, all participating faculty have agreed to these terms in order to include as many interested students as possible.

Joint Research Projects

1. **Novel Functional Materials:** There is a need for novel functional materials in the area of solar energy conversion. Points of inclusion are:

- Judicious control of electronic and charge-transport properties (possibly through self-ordering)
- Easily processable materials with consistent properties and purity
- Nontoxic materials, synthesized from abundant elements.
- High photo and redox stability (mixed inorganic and organic)
- Modeling of relevant properties in solution and in the solid state

2. **Device Engineering:** In order to effectively use the materials and obtain the full potential of their properties, innovated techniques must be employed. These techniques include:

- Methodology to investigate and control the factors that influence open circuit voltage, short circuit current, and fill factor.
- Development of novel techniques for understanding the interplay of material workfunctions, HOMO-LUMO gap and position in devices.
- Correlation of the morphology of interfaces with their observed charge transfer rates.

Working Group 3: Nanomaterials and the Environment- A

Andrew Maynard, Wilson Center – *Co-leader*

Hui-Ming Cheng, Institute of Metal Research, CAS - *Co-leader*

Robert Hurt, Brown University - *Scribe*

Richard Flagan, Caltech

Feiyu Kang, Tsinghua University

Paige Wiecinski, University of Wisconsin - *Student*

Giri Gururajan, University of Delaware - *Student*

Dhimiter Bello, University of Massachusetts, Lowell (day 2)

Process

- The group focused on environmental challenges associated with nanostructured materials, and used these as a basis for discussing collaborative synergies, opportunities and barriers.
- Three “big ideas” were developed through the discussions. These grew from the interests and expertise of the group, and do not necessarily represent the most pressing needs and opportunities in this area.
- Particular attention was paid to the question “why initiate collaborations between the US and China?” Ideas for collaborative research were explored where there appeared more to be gained from international collaboration than from each country working in isolation.
- Many of the advantages associated with collaborations between the US and China in the area of environmental impacts and benefits were common to the three big ideas explored.
- It was generally felt that the barriers to collaborating between established disciplines were greater than those affecting international collaborations in the same discipline.

Key advantages to US-China collaborations in the area of the environment

- Mutual transfer of information along knowledge-gradients (filling in knowledge gaps in each country). Driven by differences in level of knowledge, expertise and experience in the US and China in the area of nanostructured materials and the environment provide fruitful grounds for mutually beneficial collaborations
- Global challenges need global solutions. It makes good sense to ensure the US and China—two of the world’s largest economies—are following parallel tracks when it comes to reducing/managing environmental impact. This topic is especially attractive for international collaboration due to its intrinsically non-competitive nature.
- Global commercial markets for nanostructured material-based products will require international consensus on how to develop the underlying technologies responsibly and move toward harmonization of standards.

Key Barriers to effective collaboration

- Perceptions of the importance of environmental research amongst scientists and funders
- Cross-disciplinary communication; Cross-disciplinary funding
- Funding for targeted research that leads to the application of environmentally-relevant outputs.

- Communication
- Interaction with industry
- Political/commercial constraints on international collaboration
- Culture of nanotechnology favors research based on over-hyped expectations of device breakthroughs and excludes most research on many issues critical to commercial success and long-term sustainability.

1. Recommendations (with priorities)

Near-term:

- Organize a US-China workshop on sustainable nanotechnologies
- Create a working group on environmental nanomaterial measurement and characterization technologies
- Develop tools to educate the next generation of engineers for the rational design and operation of economic, safe, and sustainable nanomanufacturing processes.

Long-term

- Use the sustainable nanotechnologies workshop to establish an International Institute for Sustainable Nanotechnology (see projects)
- Develop suite of nanoparticle detection technologies and use them to
- Characterize nanoparticle concentrations, sizes, morphologies in environmental compartments relevant to potential exposures
- Develop a mechanistic understanding of nanoparticle liberation (NLF)
- Develop systematic engineering science for designing “green” nanomanufacturing processes that will be economic, safe, and sustainable

2. Potential research projects (3 examples)

A. Organize a series of joint US-China workshops on Sustainable Development of Nanotechnologies with these features:

- focus on environmental implications (rather than environmental applications)
- focus on one materials class (e.g. carbons) per meeting or per session, where specific “stakeholders” in those materials (experts in synthesis, device development, environmental science, and health impacts) can exchange detailed scientific information (the major scientific questions on toxicity, safe design, and even exposure are material-specific)
- deal with full range of issues, including exposure, toxicity, life-cycle analysis, and safe design strategies
- reach concrete conclusions (and a product) about prospects and research directions.

Use the workshop to develop plans for a permanent *International Institute for Sustainable Nanotechnology Development*, through the IMI program, or another special funding mechanism, as a world-wide hub of exchange and cooperation.

B. Initiate a joint US-China project on nanomaterial liberation, detection and quantification

- Focus on nanomaterials in environmental samples (air, soils, water, sediments, surfaces) and products.
- Three elements: detection methodologies, physics of nanomaterial release, characterization of nanomaterials in all relevant environmental media.
- Priorities: air in workplace, contact exposure (workplace and consumer use)
- The joint project will catalyze international effort and cooperation will speed progress nanomaterial safety is in both countries' interest (import / export) and the collaboration is not overly complicated by IP issues
- Exploit synergies by tapping into complementary Chinese and US research strengths, including strong Chinese efforts on scalable nanomaterial synthesis and near-term commercial materials (e.g. MWNTs) that form good test cases for environmental effects; US-NSF focus on fundamental science (aerosols, colloids, detection methodologies).

C. Initiate joint projects on green nanomanufacturing. Focus on the scientific issues arising in the systematic design of environmentally benign nanoproducts and nanoprocesses. The projects could center on specific material case studies, and consider:

- Process engineering science for nanofabrication. Apply and adapt chemical engineering paradigms to nanomaterial production.
- Educate the next-generation of engineers in benign nanofabrication.
- Manufacturing safety
- Nano-pollution control and prevention (replacement of hazardous solvents, intermediates, product toxicity control)
- Life-cycle analysis (incl. carbon footprint, impact on water resources)
 - Effective large-scale nanomanufacturing will be key for the long-term success of the nanotechnology movement, especially in this era of diminishing resources and global environmental impact.
 - US-China collaboration will help catalyze international response to this global issue

4. The Big Picture

a. US-China leadership in global energy and environmental challenges

b. Vision and mission (e.g. the establishment of a Global E institute)

Working Group 4: Nanomaterials and the Environment – B

Mamadou Diallo, Caltech (US) – *Co-leader*

Jian Xu, Institute of Chemistry, CAS (China) – *Co-leader*

John Rabolt, University of Delaware (US) - *Scribe*

Kimberly Gray, Northwestern University (US)

Gang Bao, Michigan State University (US)

Duan Weng, Tsinghua University (China)

Shu-Feng Hsieh, University of Massachusetts, Lowell (US) - *Student*

Aihui Yan, Brown University (US) - *Student*

Part 1: Improving Collaborations

1. Barriers

- Travel VISAs
- Distance
- Nomenclature: Nanomaterials vs Nanoscale Materials
- IP – this may be large barrier; Export control issues
- Cultural: language, regulatory environment
- Pressure to commercialize; conflict between basic and applied research
- Differing funding mechanisms
- Educational protocols; institute vs. university-centric training
- Research drivers: national research priorities vs. investigator initiated. Different incentives for collaboration: in China it is exchange of ideas, in U.S., it is driven by other motives, e.g., funding availability and interdisciplinary activities
- Interdisciplinarity: Different modes of operation

2. How can barriers be overcome – train students earlier, student exchange, establish long-term connections, build connections over time, emphasize sustainability of relations, deeper knowledge, acknowledge different work/education cultures. Keep collaborations on fundamental science – keep IP and commercialization in perspective.

3. Complementary strengths – need to identify focus areas; Good opportunity for collaboration within China and US to integrate material synthesis, structure, function, & theory, computation; Shared facilities – for example Advanced Photon Source in US; identify gaps in complementary user facilities (e.g., neutron/x-ray sources, etc.) that are available for collaborative research

4. Improve networking – facilitate travel by U.S. scientists and students to attend China conferences/workshops to become more acquainted with facilities and processes of collaboration; encourage longer term visits, establish collaborations over extended periods

Part 2: Joint Research Projects

General thoughts:

- Nanomaterial/technology, concentrate on science
- Big drivers – water and energy; also air; CO₂ emissions, real-time environmental sensing, monitoring and remediation
- Nanotechnology will allow distributed power and water treatment systems for the public sector
- Green, environmentally benign, eco-friendly materials –does not have a lot of traction in U.S.

- Minimize emissions – ideally, nanotechnology can be part of the solution; e.g. – Hg and coal – how to capture, but final disposal still problem.
- Nanotechnology – membranes, (smart membranes with embedded sensors, actuators to modify pore and tune selectivity).

Specific Research Projects: Multi University/Institute Research Initiatives Model

1. Multifunctional Membranes from Nanofibers
Collaborating Institutions: CAS, Caltech, Tsinghua, Delaware
2. Transparent Surface Coating with Nanostructure and Anti-reflection Properties
Collaborating Institutions: CAS, Michigan State, Tsinghua, UCLA
3. Structure, Processing and Properties of Polymer Nanofibers for Light Sensing, Sound Absorbance and Filtration
Collaborating Institutions: Delaware, Michigan State, Caltech, CAS

Project 1: Transparent surface coating with nano-structure and anti-reflection properties

Rationale: With the development of global industrialization processes, energy demand for human is growing increasingly. Since solar energy is an inexhaustible energy supply, research on the use of solar energy aroused a great deal of attention of a lot of researchers. However, the shortage of silicon materials and high cost for fabricating solar cell restricts the application of solar cell in our lives greatly. Antireflective coatings on surfaces not only can improve the transparency of optical devices, but also can increase the photovoltaic conversion efficiency of solar cell materials. Employing antireflective coating in solar cell field is simple and effective method to solve the two problems above mentioned in photovoltaic solar cell field. Here, we developed a facile method for fabricating antireflective silica film with nanoporous structure, which can increase the power of solar cells effectively.

The uniform film were composed of nanoparticles about 20~30 nm and nanopores formed by the accumulation of nanoparticles. It is believed that nanopores formed by nanoparticle assembly increased the surface roughness and further promoted its hydrophilicity. The coated glass slides have also a better light transmittance.

Computational modeling provides significant challenges since the model problem is of multiscales and of limited computational resources.

Goals: Based on the nano-structure, the light transmittance of the coated glass slide is up to 92%~ 97% in the visible light range (390~780nm) and 95% ~ 97 % in the major visible light range(460~750). That above-mentioned indicated that the as-prepared film can improve the light transmittance of substrate material. Another objective to develop computational models and tools for systematic designs and modeling of the intended nano structures.

Required expertise and participating institution in US and China

Jian Xu, ICCAS of CAS and Prof. Duan Weng of Tsinghua University corporate with Prof, Yang Yang at UCLA and Prof. Gang Bao at Michigan State University.

Collaboration structure: US Institutions and Institute of Chinese Academy of Sciences

Complementary facilities and capabilities

Prof. Xu's group can prepare the nano-particles made of inorganic-organic nanoparticle and cast the homogeneous film, which the thickness is controlled in 100-200 nm. Prof. Yang can studies the materials and assembly solar cell, and Prof. Bao's group will develop modeling and computation tools to guide real experiments and analyze the results.

Anticipated outcomes

A transparent surface coating on solar cell glass with anti-reflection behaviors can be used in solar cell, which enhances effectively the light transparency from 91% to more than 95%. It means the cell yield of solar light-electronic power transfer increases about 0.3-0.5% on the present data.

3-5 published papers

Broader impact including integration of research with education

Exchange Ph.D students or postdoctoral fellows between ICCAS and UCLA and MSU

Budget consideration

\$1,000,000-2,000,000 annually supported by both NSF and NSFC

Project 2: Structure, Processing and Properties of Polymer Nanofibers for Light Sensing, Sound Absorbance and Filtration

Rationale: Air, water, soil and noise pollution are systemic problems that affect daily living in all cultures throughout the world. For example, noise pollution can cause noise-induced hearing impairment; interference with speech communication; disturbance of rest and sleep; mental-health deterioration and job-related performance issues, etc. Hence, developing new, low cost, multifunctional, nanoscale materials and processes to sequester contaminants and to control noise pollution would address an important issue in improving the quality of life. Current strategies are either marginally effective, costly or both. There is a need for a room temperature, electrostatic shaping of polymers (electrospinning) in concert with electric field induced nanofiber collection to produce a new generation of multifunctional membranes that are responsive to contaminants and provide noise-absorbance characteristics that are superior to those that currently are in use. In addition, a critical need exists for a simple, high rate toxicity screening of nanofibers (nanoparticles, nanotubes) and the effect of environmental release. Biological oxidative stress (BOS) is implicated in many diseases and is a principal mechanism of toxicity. Hence, the potential toxicity and environmental impact of these nanofibers have to be carefully evaluated before large-scale applications are undertaken.

Goals: To understand the relationship between the structure (molecular, crystal and morphological), processing and properties of polymer nanofibers so as to be able to optimize their performance in sensing, absorbance and filtration applications. Develop a room-temperature electrospinning process that allows the incorporation of "guest" molecules into the nanofibers with a subsequent migration to the surface so as to sequester contaminants, absorb/reflect light or reduce sound.

Required expertise and participating institutions in US and China: Synthesis of novel multifunctional polymers (CAS); Nanofiber processing and characterization (Delaware, Caltech);

Membrane synthesis and testing (Caltech, Delaware, CAS), Materials modeling (Caltech); toxicity and environmental impact (Brown, UMass).

Collaboration structure: Multi-university research initiatives (MURI) model.

Complementary facilities and capabilities: Polymer nanofibers will be prepared as films and membranes and characterized (IR, Raman x-ray, Neutron scattering, SEM) for applications ranging from sensing to filtration (US, China). Incorporation of thermochromic, photochromic and solvatochromic dyes into these fibers during the room-temperature fabrication stage can provide a “smart” component to the sensing mechanism (US). Fiber diameters can be controlled and generally will be in the 100-1000 nm. range. The sound absorbance capabilities of the polymeric membranes fabricated from either native or “filled” polymer fibers will be investigated and their mechanical, thermal and electronic properties optimized for use as “smart” sensors (China)). Multifunctional materials (small molecules and oligomers, etc.) for incorporation into the polymer nanofibers so that they can be used for the sequestration of contaminants (metals, bacteria, viruses, etc.) in water and air (US). Parallel studies of toxicity of the nanofibers produced will be undertaken in both the US and China.

Anticipated outcomes: Understand critical processing parameters necessary for molecular alignment of polymer chains in nanofibers so as to manipulate their mechanical, optical and thermal properties. Produce multifunctional, nanofibrous membranes for sequestration of contaminants from water, soil and air. Create underlying knowledge for “smart” membrane sensors. 8-10 papers/yr published in high impact, peer reviewed journals.

Broader impact including integration of research with education: Creation of a small company to commercialize functionalized, nanofibrous membranes; Cross-technical and cultural training of Ph.D students and/or postdoctoral fellows in the correlation of structure, processing and properties of polymer nanofibers.. Students will be trained to work in multinational, multidisciplinary teams, a critical skill set for employment in global companies.

Budget considerations: \$800,000-\$1,300,000 annually supported by both NSF and NSFC

Project 3: Multifunctional Membranes from Nanofibers

Rationale: Membranes are key components of a variety of environmental and industrial processes including water treatment, gas separation and air pollution control. Current polymeric and ceramic membranes are not very selective, require high pressure to operate and are prone to loss of performance overtime due to fouling and degradation. Nanofibers are emerging as building blocks for novel and more effective filtration media. However, the science underlying the fabrication, operation and potential environmental impact of nanofiber-based membranes is not well understood.

Goals: The overall objective of this project is to develop structure-properties relationships that can be used to guide the design fabrication of novel nanofiber-based membranes for water treatment and gas separation

Required expertise and potential participating institutions in US and China: Nanofiber synthesis and characterization; Membrane fabrication and testing; Multiscale modeling; Environmental impact assessment

Collaboration structure: Similar to DOD Multi-University Research Initiative (MURI) (3 American PI and 3 Chinese PI) 3 Years initial funding + 2 years renewable

Complementary facilities and capabilities: Polymer and nanofiber synthesis and characterization lab; Membrane fabrication and filtration lab; Multiscale materials simulation hardware and software; Environmental chemistry and biology lab

Anticipated outcomes: Develop the science needed for the rationale design and fabrication of nanofiber-based water treatment and gas separation membranes; Enhance scientific collaboration/exchange between US and China

Broader Impact

Develop a new generation of more efficient water and gas separation membranes.

Provide students with multidisciplinary training opportunities

Enhance US-China research/education cooperation in science and engineering

Budget considerations: \$ 1 Million per year (US) + \$1 Million per year (China)

Action items: Follow-up activities by US NSF and NSFC to move project forward

Working Group 5: Novel synthesis and characterization

Isiah Warner, Louisiana State University (US) – *Co-leader*

Jiaguo Yu, Wuhan University of Technology (China) – *Co-leader*

Theodore Goodson, III, University of Michigan (US) – *Scribe*

Gerald Young, University of Akron (US)

Dhimiter Bello, University of Massachusetts Lowell (US)

Olivia Graeve, Alfred University (US)

Yichun Liu, Northeast Normal University (China)

Raghunath Kanakala, Alfred University (US) - *Student*

1. Recommendations (with priorities)

Near-term

- Create a searchable table which has particular expertise of institutions in china so that one can swiftly locate key places to determine potential interests and thus collaborations. Ask NSFC for a searchable database of potential collaborators
- Must have a human connection in order to really begin a collaboration. Obtain some small seedling or travel grant to visit.
- Possible visit international meetings in china (MRS-China) in order to get to know scientists in china.
- Make it clear that there is an interest in joint publications and potentially joint grant submission.

Long-term

- Reduce political differences and barriers for good cooperation!
- Discussions about “limited” export of technology from the USA to China, in order to define some clear benefits toward the realization of a larger or broader scale collaboration and benefits.
- Consider reducing the burden of cost by the Chinese colleagues by helping to pay for students and faculty visiting and setting up infra-structure for collaboration.
- EXCHANGE of students is important, in other words it is also important for our students to train abroad. The ratio of exchange of students is lop-sided. Encouragement from advisors and mentors for students to go abroad.
- Long term partnership between particular universities in the USA with complimentary universities in china forming a network (small at first) that can develop a pipeline and ongoing collaboration with mutual goals.
- Identify former students and postdocs who are now faculty or administrators in china institutions (or students from china who are now faculty in the USA) who might want to setup a network or a part of the network of collaboration.

2. Research Collaborations

a. Barriers to US-China collaboration

- Distance
- Language

- Sharing of Intellectual property
 - Research support, facilities and Level not on equal ground in some respects.
 - Complimentary resources and facilities are not always available in china.
 - Identifying people and projects which are compatible to the projects
 - Visa status is difficult to get or not in a timely manner especially for collaboration basis and not for Ph.D. in the united states.
 - Is basic research a focus at collaborating institution?
 - 4 billion budget for all scientific research and 33% is used for medical research. The money has to cover a lot of ground.
 - Competition from European union collaborators
 - Transferring of data, materials, and property with china (and other countries) can be difficult at times and limit a good collaboration.
 - Need a two-way street (driving force) toward setting up infra-structure for making fruitful collaborations.
 - Cultural differences in doing interdisciplinary research at collaborating institution.
- b. Common strengths and attributes which can be used to overcome barriers**
- Educational system and development of students
 - At the undergraduate level, very strong in basic mathematics and science
 - Students in china have a great deal of drive and determination and the US top students are just as good.
 - China offers access to unique populations and problems in comparison to the US.
 - Willingness on both sides for investments in human capital in training and motivating students, building infrastructure, and using real financial resources.
 - Use of materials research institutes toward setting up the infra-structure for broad base and fruitful collaborations.
 - Science in an international language
 - Size is a big advantage (two big countries with lots of researchers), can cover a lot of ground with a lot of people, but also have to pick the right direction in the end.
 - The existence of “SBIR” type mechanisms in both countries
- c. Suggestions for improving networking**
- More targeted workshops
 - more narrow scope topics.

3. Potential Research Projects

Project 1: Non-template Self-transformation Fabrication of Hollow Inorganic Microspheres and Their Application in Water and Air Purification

Potential collaboration with engineer/materials science to carry out the fabrication of a real device to test the purification procedure. Dr. Jioguo Yu, Prof. Kimberly Gray with other interested collaborators. The collaboration may be an independent collaboration at first, however one can see how this might be scalable in to a larger structure with the ever present problem of water filtration.

Project 2: Investigations of High Dielectric Constant Effects in Pthalocyanine systems.

Rationale: Novel pthalocyanine systems have shown great promise for high dielectric effects due to the long range delocalization in extended systems. This effect can be utilized to produce high dielectric constants at higher frequencies. There is still much to be learned regarding the mechanism and nature of the structure-function relationships in functionalized pthalocyanine systems. Dr. Liu will prepare the novel pthalocyanine materials and Dr. Goodson will do dielectric and optical measurements on the materials.

Goal: Obtain a set of parameters related to the functionalization of pthalocyanine nanomaterials and dielectric properties and to use a number of spectroscopic topics to probe the mechanism of electron and energy transfer in these materials.

Complementary Expertise in the US and China: Dr. Yun Qi Liu Chinese Academy of Sciences and Theodore Goodson III, University of Michigan. Dr. Liu has extensive expertise in synthesis of novel organic materials. Dr. Goodson has extensive expertise in optical and electronic properties of organic and nanostructured materials.

Operation: After initial collaboration discussions and perhaps initial measurements of start materials, the PI's will seek seedling funding to meet and to interact face to face and to see eachother's laboratory and research groups. After this, if successful, one can see the need for further collaboration in to making specific devices (for example) as well as microscopic (nanoscopic) investigations for surface morphology of thin films with this material. This may be an avenue to the creation of a smaller network of collaborating research groups which might later constitute the genesis of a international materials research institute.

Broader impact of educating students who would have only had the opportunity to see one aspect (synthesis or measurements) of the research to see both and how the materials might later be used for real applications. This fosters interdisciplinary research. It might suggest that the probability of success of solving such problems in a more timely manner possible with the combined expertise and collaboration. Finally, exposing students to other cultures (and work habits) might enhance the general education and mentorship of the students in both countries. China is starting to offer support to students and postdocs who seek interdisciplinary training in various areas of materials and environmental science. This may reduce the language barrier (perhaps within the next ten years) due to rapid exchange of students and expertise in these collaborations.

4. The Big Picture

- a. US-China leadership in global energy and environment challenges
- b. Vision and mission (e.g., the establishment of a Global E Institute):
 - With two large and industrial countries one could develop a “governing” institute to test models and theories regarding global warming, pollution as well as other public health and technology issues.
 - Remove political stumbling blocks so that a real discussion to solve problems can take place between the two countries.