

Final report

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International Symposium on Clusters and Nanomaterials

(Energy and Life Sciences Application)

October 26-29, 2015

Richmond, Virginia Commonwealth University

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Summary

The International Symposium on Clusters and Nanomaterials was held in Richmond, Virginia during October 26-29, 2015. The symposium focused on the roles clusters and nanostructures play in solving outstanding problems in clean and sustainable energy and life sciences applications; two of the most important issues facing science and society. Many of the materials issues in renewable energies, environmental impacts of energy technologies as well as beneficial and toxicity issues of nanoparticles in health are intertwined. Realizing that both fundamental and applied materials issues require a multidisciplinary approach the symposium provided a forum by bringing researchers from physics, chemistry, materials science, and engineering fields to share their ideas and results, identify outstanding problems, and develop new collaborations.

Clean and sustainable energy sessions addressed challenges in production, storage, conversion, and efficiency of renewable energies such as solar, wind, bio, thermo-electric, and hydrogen. Environmental issues dealt with air- and water-pollution and conservation, environmental remediation and hydrocarbon processing. Topics in life sciences included therapeutic and diagnostic methods as well as health hazards attributed to nanoparticles. Cross-cutting topics such as reactions, catalysis, electronic, optical, and magnetic properties were also covered.

The symposium attracted 132 participants from 24 countries in the world. It featured 39 invited speakers in 14 plenary sessions, in addition to one key-note session. Eighty-five contributed papers were presented in two poster sessions and 14 papers from this list were selected to be presented orally at the end of each session to highlight hot topics. Papers presented at the symposium were reviewed and published in SPIE so that these can reach a wide audience. The symposium was highly interactive with ample time allotted for discussions and making new collaborations. The participants' response was that this was a high quality conference and covered topics at the cutting edge of science and technology.

The symposium was endorsed by the American Physical Society, The Materials Research Society, SPIE, The Metallurgical Society, and the American Vacuum Society.

The symposium was supported by external grants from the National Science Foundation and the Department of Energy as well as by internal grants from Virginia Commonwealth University (Offices of the President, Provost and Vice President of Academic Affairs, Vice President of Research, Vice Provost for Life Sciences, Dean of the College of Humanities and Sciences, and the Dean of the School of Engineering). The funding from DOE was used to support partial expenses of invited speakers, students and postdoctoral fellows.

Topics covered at the symposium

The topics dealt with the role of clusters and nanostructures (nanowires, nanotubes, nanoparticles, quantum dots, and monolayers such as graphene and beyond) in solving outstanding problems in energy and life sciences.

Clean and sustainable Energy: Production, Storage, Conversion, and Efficiency

Solar

Hydrogen

Energy Storage Systems (nanostructured electrodes, batteries)

Thermo-electrics

Photothermal Energy Conversion

Life Sciences: Bioactive, bio responsive, and biomimetic materials, nano-toxicity, bio engineering and regenerative medicine, Diagnostics (sensors, image enhancement), Therapeutic (drug design and delivery, non-invasive cancer treatment), safer-by-design.

Cross-cutting Topics: NanoCatalysis (eg. new developments in core-shell catalysts), Properties (Electronic, Optical, and Magnetic), hybrid nanoparticles, carbon nanostructures, polymer nanoparticles, and nanoparticle ferrofluids.

Organization

Chairman: Puru Jena, Virginia Commonwealth University

Secretary: Anil K. Kandalam, West Chester University of Pennsylvania

International Advisory Board:

Barbara D. Boyan, Virginia Commonwealth University (USA)

Catherine Bréchnac, CNRS (France)

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Zhongfan Liu, Peking University (China)

Chad A. Mirkin, Northwestern University (USA)

Risto M. Nieminen, Aalto University School of Science and Technology (Finland)

C.N.R. Rao, Jawaharlal Nehru Centre for Advanced Scientific Research (India)

Gabor A. Somorjai, University of California Berkeley (USA)

John T. Yates Jr, University of Virginia (USA)

Organizing Committee:

Pulickel M. Ajayan, Rice University (USA)

Kit H. Bowen, Jr., Johns Hopkins University (USA)

Chris M. Cannizzaro, U. S. Department of State (USA)

Hani El-Kaderi, Virginia Commonwealth University (USA)

Mohamed S. El-Shall, Virginia Commonwealth University (USA)

Diana Farkas, Virginia Tech. (USA)

Joseph Poon, University of Virginia (USA)

Subhendra D. Mahanti, Michigan State University (USA)

James T. McLeskey, Jr., Virginia Commonwealth University (USA)

Jason C. Reed, Virginia Commonwealth University (USA)

Joseph S. Reiner, Virginia Commonwealth University (USA)

Qiang Sun, Peking University (China)

Sally S. Tinkle, Science and Technology Policy Institute (USA)

SCIENTIFIC PROGRAM

Sunday, October 25

5:00 – 8:00 PM **Registration**, Rotunda, Jefferson Hotel
7:00 – 8:00 PM **Reception**, Rotunda, Jefferson Hotel

Monday, October 26

INAUGURAL SESSION

9:00 – 9:10 AM Introductory Remarks
 Puru Jena, Symposium Chair, Virginia Commonwealth University, USA
9:10 – 9:20 AM Welcome Address
 Michael Rao, President, Virginia Commonwealth University, USA

KEY NOTE ADDRESS

9:20 – 10:05 AM “Nanowires, Nanoelectronics and the Interface with Biological Systems”
 Charles M. Lieber, Harvard University, USA

10:05 – 10:30 AM **COFFEE BREAK**

Session A: CATALYSIS-I

Chairman: Samy El-Shall, Virginia Commonwealth University, USA

10:30 – 11:00 AM “Molecular catalysis science: Nanoparticle synthesis and instrument development for characterization under reaction conditions - Conquering catalytic complexity”
 Gabor A. Somorjai, University of California, Berkeley, USA
11:00 – 11:30 AM “Nanostructured Materials for Energy and Green Chemistry Applications”
 Jackie Y. Ying, Institute of Bioengineering and Nanotechnology, Singapore
11:30 – 12:00 Noon “How do Metal Oxides Activate Methane? A Mechanistic Exercise”
 Helmut Schwarz, Technische Universität, Berlin, Germany
12:00 – 12:15 PM **Hot topic:** “Investigation of Lattice Displacement Dynamics and Nanocatalytic Activity of Gold”, **Kiran Sasikumar** and Subramanian Sankaranarayanan, Argonne National Laboratory, USA
12:15 – 2:00 PM **LUNCH**

Session B: LIGHT HARVESTING

Chairman: James T. McLeskey, Randolph-Macon College, USA

2:00 – 2:30 PM “Looking Beyond Plasmonics. Exploring Light Harvesting Properties of Glutathione Stabilized Gold Clusters ”
 Prashant V. Kamat, University of Notre Dame, USA
2:30 – 3:00 PM “Photocatalysis on TiO₂: Insights from first principles simulations”

Annabella Selloni, Princeton University, USA

3:00 – 3:30 PM

“Impurity Clusters and the Birth of Abnormal Alloys”

Angelo Mascarenhas, National Renewable Energy Laboratory, USA

3:30 – 3:45 PM

Hot topic: “A new class of super-ion inspired hybrid perovskites for solar cells”,
Hong Fang and Puru Jena, Virginia Commonwealth University, USA

3:45 – 4:15 PM

COFFEE BREAK

Session C: BEYOND GRAPHENE

Chairman: Qiang Sun, Peking University, China

4:15 – 4:45 PM “Nanowires of aluminum hydroxide (boehmite: γ -AlO (OH))”

Sumio Iijima, Meijo University, Japan

4:45 – 5:15 PM

“New Metastable Phases of Carbon”

Qian Wang, Peking University, China

5:15 – 5:45 PM

“Graphene and Beyond: Attraction, Reality and Future”

Zhongfan Liu, Peking University, China

5:45 – 6:00 PM

Hot topic: “Solution Chemical Syntheses of 2D Tin Chalcogenide Nanoscale Device Components”, **Adam J. Biccchi**, Joseph A. Hagmann, Son T. Le, Sugata Chowdhury, Curt A. Richter, and Angela R. Hight Walker, National Institute of Standards and Technology, USA

6:00 – 8:00 PM

DINNER

8:00 – 10:00 PM

POSTER SESSION – I, Empire Room

Tuesday, October 27

Session D: BIO-INSPIRED & BIO-COMPATIBLE MATERIALS

Chairman: Jason Carlyon, Virginia Commonwealth University, USA

8:30 – 9:00 AM

“Semiconductor Nanomaterials for Electronics That Can Dissolve in Your Body”

John A. Rogers, University of Illinois, Urbana, USA

9:00 – 9:30 AM “Protein-based hybrid materials: towards sustainable hydrogen production”

Giovanna Ghirlanda, Arizona State University, USA

9:30 – 10:00 AM

“Nanoparticle Biocompatibility: Lessons Learned from the NCL”

Scott E. McNeil, Frederick National Laboratory, USA

10:00 – 10:15 AM

Hot topic: “Multi-Stimuli Responsive Drug Delivery using Polypyrrole Nanoparticles”, **Devleena Samanta**, Stanford University, USA, Jana L. Meiser,

Leibniz Universität Hannover, Germany, Niloufar Hosseini-Nassab, Stanford University, Daphney Sihwa, Spelman College, Atlanta, Evgenios Neofytou, & Richard N. Zare, Stanford University, USA

10:15 – 10:45 AM **COFFEE BREAK**

Session E: CLUSTERS - I

Chairman: Kit Bowen, Johns Hopkins University, USA

10:45 – 11:15 AM “Boron Clusters: From 2D Clusters to Borophene and Borospherene”
Lai-Sheng Wang, Brown University, USA

11:15 – 11:45 AM “Gold and Silver in Nanoscale, Dispersed by Ligands to Molecular Precision”
Hannu Hakkinen, University of Jyväskylä, Finland

11:45 – 12:15 PM “Gas phase-Infrared-Photo-dissociation Spectroscopy of Carbon Anion Species of Astrophysical Relevance”
Ludger Wöste, Freie Universität, Germany

12:15 – 12:30 PM **Hot topic:** “Excited state lifetimes of metal clusters”, **G. Ganteför**, University of Konstanz, Konstanz, Germany and W. Eberhardt, TU Berlin, Germany

12:30 – 2:30 PM **LUNCH**

Session F: ENERGY STORAGE & CONVERSION

Chairman: Jagjit Nanda, Oak Ridge National Laboratory, USA

2:30 – 3:00 PM “Subnanometer metal clusters as catalysts in Li-O₂ batteries”
Larry Curtiss, Argonne national Laboratory

3:00 – 3:30 PM “Role of Nanomaterials in Next Generation Battery Chemistries”
Arumugam Manthiram, University of Texas at Austin, USA

3:30 – 4:00 PM “Complex Hydrides for Energy Device Research”
Shin-ichi Orimo, Tohoku University, Japan

4:00 – 4:15 PM **Hot topic:** “Achieving High Thermoelectric Figure of Merit in Nanostructured Half-Heulser Alloys”, **Joseph Poon**, Long Chen, Sheng Gao, University of Virginia, and Xiaoyu Zeng, A. M. Dehkordi, Terry Tritt, Clemson University, USA

4:15 – 6:15 PM **FREE TIME/NETWORKING**

6:15 PM **Group Photo, Grand Stair Case, Jefferson Hotel**

6:30 PM **RECEPTION, Rotunda, Jefferson Hotel**

7:00 PM

Banquet: Ball Room, Jefferson Hotel

After-Dinner Speaker: Lloyd Whitman, White House Office of Science and Technology Policy, Washington D.C., USA

Wednesday, October 28

Session G: CATALYSIS - II

Chairman: Olof Echt, University of New Hampshire, USA

- 8:30 – 9:00 AM “Catalysis in confined space – from zeolites and zeotypes to functionalized metal-organic frameworks”
Unni Olsbye, Oslo University, Norway
- 9:00 – 9:30 AM “Descriptor based Design of Catalytic Nanoalloys and Clusters using Density Functional Theory and Genetic Algorithms”
Tejs Vegge, Technical University of Denmark, Denmark
- 9:30 – 10:00 AM “Cluster modeling of water oxidation in photosystem II ”
Per E.M. Siegbahn, Stockholm University, Sweden
- 10:00 – 10:15 AM **Hot topic:** “Dendrimer-mediated Transformation of the Intracellular Bacterial Pathogen, *Anaplasma phagocytophilum*”, **Aminat T. Oki**, David Seidman, Michael G. Lacina III, Hu Yang, Jason A. Carlyon, Virginia Commonwealth University, USA
- 10:15 – 10:45 AM **COFFEE BREAK**

Session H: CLUSTERS - II

Chairman: Gerd Gantefor, University of Konstanz, Germany

- 10:45 – 11:15 AM “Fulfilling Feynman's vision: arranging the atoms in size-selected clusters with multiple applications”
Richard E. Palmer, University of Birmingham, UK
- 11:15 – 11:45 AM “Functionality of Small Metal Clusters: From Basics towards Sensors and Selective Catalysis”
Vlasta Bonacic-Koutecky, Humboldt University, Germany
- 11:45 – 12:15 PM “Structure, Stability, Physical and Chemical Properties of Small Gold Clusters and their Alloys”
Peter Lievens, KU, Leuven, Belgium
- 12:15 – 12:30 PM **Hot topic:** “Thiolated Gold Nanomolecules”, **Amala Dass**, University of Mississippi, Oxford, USA
- 12:15 – 2:30 PM **LUNCH**

Session I: BIOMIMETIC MATERIALS
Chairman: Sally Tinkle, Science and Technology Policy Institute, USA

- 2:30 – 3:00 PM “Harnessing Biomimetic Catch Bonds to Create Mechanically Robust Nanoparticle Networks”
Anna Christina Balazs, University of Pittsburg, USA
- 3:00 – 3:30 PM “Toward an Understanding of Crystallization by Particle Attachment in Biologic, Geologic, and Synthetic Systems”
Patricia Dove, Virginia Tech, USA
- 3:30 – 4:00 PM “Assembly of Nanoparticles and Chiral Nanomaterials”
Nicholas A. Kotov, University of Michigan, USA
- 4:00 – 4:15 PM **Hot topic:** “Micropatterned Functional Biomimetic Architectures”, **Ramendra K. Pal**, Nicholas E. Kurland, Ahmed A. Farghaly, Maryanne M. Collinson, Vamsi K. Yadavalli , Virginia Commonwealth University, USA
- 4:15 – 4:45 PM **COFFEE BREAK**

Session J: CLUSTER ASSEMBLIES
Chairman: Amal Dass, University of Mississippi, USA

- 4:45 – 5:15 PM “Mathematical Control in the Self-assembly of Giant M_nL_{2n} Polyhedral Clusters”
Makoto Fujita, The University of Tokyo, Japan
- 5:15– 5:45 PM “Electronic Structure, Assembly, and Chemistry of Precise Clusters”
Paul S. Weiss, University of California - Los Angeles, USA
- 5:45 – 6:15 PM “Modulation of complex neuronal cell activities by mechanotransductive signaling induced by surfaces with engineered nanoscale roughness”
Paolo Milani, University of Milano, Italy
- 6:15 – 6:30 PM **Hot topic:** “Brewing Metal-Organic Chalcogenide Assemblies (MOCHA) using Molecular Self-Assembly”, **J. Nathan Hohman**, Lawrence Berkeley Laboratory, USA
- 6:30 – 8:30 PM **DINNER**
- 8:30– 10:00 PM **POSTER SESSION – II, , Empire Room**

Thursday, October 29

Session K: HYDROGEN and ELECTROCHEMICAL STORAGE
Chairman: Ragaiy Zidan, Savannah River National Laboratory, USA

- 8:30 – 9:00 AM “Borohydrides as Energy Storage Materials”
Arndt Remhof, Empa, Zutich, Switzerland
- 9:00 – 9:30 AM “Multi-functional Energy Storage Materials”
Torben Jensen, Aarhus University, Denmark
- 9:30 – 10:00 AM “Hydrogen Compounds- A Brilliant Bridge to Magnesium Batteries”
Rana Mohtadi, Materials Research Department Toyota Research Institute of North America, USA
- 10:00 – 10:15 AM **Hot topic:** “Hydrogen Interaction with Carbon Nanostructures and the Formation of Novel Materials”, **Ragay Zidan**, Joseph A. Teprovich Jr., Patrick A. Ward, and Aaron L. Washington, Savannah River National Laboratory, and Puru Jena, Virginia Commonwealth University
- 10:15 – 10:45 AM **COFFEE BREAK**

Session L: BIOMATERIALS
Chairman: Jason Reed, Virginia Commonwealth University, USA

- 10:45 – 11:15 AM “Surface affinity: Applications of a functional assay for quantifying nanoparticle transport, aggregation, transformation and biouptake in complex systems”
Mark Wiesner, Duke University, USA
- 11:15 – 11:45 AM “How Nanostructural Features of a Biomaterial Regulate Musculoskeletal Cells and Tissues”
Barbara Boyan, Virginia Commonwealth University, USA
- 11:45 – 12:00 PM **Hot topic:** “Computational Design of SWCNT-Cisplatin-like Nanodevices and a Model for their Interaction with Certain Overexpressed Proteins in Ovarian Cancer”, Erik Díaz-Cervantes^{a,b} Miquel Solà^b Marcel Swart^{b,c} and **Juencio Robles^{a,*}** Universidad de Guanajuato, México; ^b Universitat de Girona, Spain; ^cInstitució Catalana de Recerca i Estudis Avançats, Barcelona, Spain.
- 12:00– 2:00 PM **LUNCH**

Session M: THERMOELECTRIC MATERIALS
Chairman: Joe Poon, University of Virginia, USA

- 2:00 – 2:30 PM “Phonon Transport in Nanostructures: Ballistic, Coherent, and Hydrodynamic Modes”
Gang Chen, Massachusetts Institute of Technology, USA
- 2:30 – 3:00 PM “Nanostructures in Thermoelectrics – recent advances and understanding”
Subhendra D. Mahanti, Michigan State University, USA

- 3:00 – 3:15 **Hot Topic: Q.** “Assembling Organic Molecules with Negative Gaussian Curvature for Ultrahigh Thermoelectric Efficiency”, Jiabing Yu and **Qiang Sun**, Peking University, Beijing, China, and Puru Jena, Virginia Commonwealth University, USA
- 3:15 – 4:00 PM “The Merging of Cluster and Nanomaterials Research Directions”
Mildred S. Dresselhaus, Massachusetts Institute of Technology, USA
- 4:00 – 4:10 PM **CONCLUDING REMARKS**
Anil K. Kandalam, West Chester University of Pennsylvania, USA

INTERNATIONAL SYMPOSIUM ON CLUSTERS AND NANOMATERIALS

Richmond, VA USA

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