SCIENTIFIC PROGRAM

SUNDAY, OCTOBER 25

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

7:00 – 8:00 PM **Reception**, Rotunda, Jefferson Hotel (Hosted by the President of VCU)

All scientific sessions will be held in the Ball Room of the 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: Sammy 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 TiO_2: 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 pervoskites 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. Biacchi, 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

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 AND CONVERSION

Chairman: Jagjit Nanda, Oak Ridge National Laboratory (USA)

2:30 – 3:00 PM	"Subnanometer metal clusters as catalysts in Li-O_2 batteries" **Larry A. Curtiss**, *Argonne National Laboratory*, USA
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 Staircase**
6:30 PM	**RECEPTION, Rotunda, Jefferson Hotel**
7:00 PM	**DINNER: 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. Lancina 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

12:30 – 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: Hani El Kaderi, Virginia Commonwealth University (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 – 10:30 PM POSTER SESSION II

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, Zurich*, 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, *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"
Ragaiy Zidan, Joseph A. Teprovich Jr., Patrick A. Ward, and Aaron L. Washington, *Savannah River National Laboratory,* and Puru Jena, Virginia Commonwealth University, USA

10:15 – 10:45 AM COFFEE BREAK

Session L: BIOMATERIALS

Chairman: Jason C. Reed, Virginia Commonwealth University (USA)

10:45 – 11:15 AM "Surface affinity: Applications of a functional assay for quantifying nanoparticle transport, aggregation, transformation and bioüptake 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 D. Boyan, *Virginia Commonwealth University*, USA

11:45 – 12:00 PM "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 **Juvencio Robles**[a] *Universidad de Guanajuato,* México; [b] Universitat de Girona, Spain; [c]Institució 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 PM	(**Hot topic)** "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 PA, USA