

SYMPOSIUM PROGRAM

Sunday, November 9

18:00 - 21:00 Registration, Submission of Manuscripts

19:00 - 21:00 Reception: Rotunda, Jefferson Hotel

**All oral presentations will be held at the Ballroom of the Jefferson Hotel.
The posters will be displayed in the Empire room.**

Monday, November 10

INAUGURAL SESSION

- 8:30 - 8:40 Introductory Remarks
P. Jena (Conference Chairman, Virginia Commonwealth University
Richmond, U.S.A.)
- 8:40 - 8:45 Welcome Address
E. P. Trani (President, Virginia Commonwealth University, Richmond, U.S.A.)

KEYNOTE SESSION

Chairman: J. R. Anderson

- 8:45 - 9:30 “To Cluster or Not to Cluster – That is the Question”
John B. Fenn, Virginia Commonwealth University, Richmond, U.S.A.
- 9:30 – 10:15 “Manipulating Atoms and Other Stuff with Light”
William D. Phillips, Natl. Inst. of Standards and Technology, Gaithersburg, U.S.A.

10:15 - 10:30 **COFFEE BREAK**

SESSION A: ATOMIC CLUSTERS

Chairman: S. Richardson

- 10:30 - 10:55 “Diffraction of Magic Helium Clusters”
J. Peter Toennies, Max-Planck-Institut für Strömungsforschung, Göttingen, Germany
- 10:55 - 11:20 “Learning About Clusters by Teaching Lasers to Control Them”
Ludger Wöste, Freie Universität, Berlin, Germany
- 11:20 - 11:45 “Experiments on Mass Selected Nanoclusters: Each Additional Atom Matters”
G. Ganteför, University of Konstanz, Germany
- 11:45 - 12:00 “Titanium Assisted Hydrogen Desorption in Alanates”
P. Jena, **S. N. Khanna**, B. K. Rao, and H. Kawamura, Virginia Commonwealth University, Richmond, U.S.A.
- 12:00 - 14:00 **LUNCH BREAK**

SESSION B: MOLECULAR CLUSTERS

Chairman: M. Kappes

- 14:00 - 14:25 “Clusters: Elucidating the Influence of Solvation on Reactions”
A. W. Castleman, Jr., Pennsylvania State University, University Park, U.S.A.
- 14:25 - 14:50 “Exploding Nanodroplets: Applications to Studies of Ion Solvation, Chemistry of Molecular Clusters, and Frontier Studies in Proteomics”
J. L. Beauchamp, California Institute of Technology, Pasadena, U.S.A.
- 14:50 - 15:15 “Factors that Affect Duplex Formation and the onset of Helix Formation in Oligonucleotides”
Michael T. Bowers, University of California, Santa Barbara, U.S.A.
- 15:15 - 15:40 “Assembly of Unsolvated Helices and Sheets into Complexes and Tertiary Structure Domains”
Martin F. Jarrold, Indiana University, Bloomington, U.S.A.
- 15:40 - 16:00 **COFFEE BREAK**

SESSION C: CATALYSIS

Chairman: A. Rosén

- 16:00 - 16:25 “Fabrication of Two-Dimensional and Three-Dimensional Platinum Nanoclusters to Serve as High Technology Catalysts – Catalysts Capable of 100% Reaction Selectivity”
G. A. Somorjai, Berkeley National Laboratory, Berkeley, U.S.A.
- 16:25 - 16:50 “Catalysis with Nanoclusters – The Role of the Nanoscale”
S. T. Pantelides, Vanderbilt University, Nashville, U.S.A.
- 16:50 - 17:15 “Remarkable Structure Sensitivity of the Catalysis by Gold Nanoparticles”
Masatake Haruta, AIST, Tsukuba, Ibaraki, Japan
- 17:15 - 17:30 “Synthesis of Nanoscale Au/Fe₂O₃ and Cu/CeO₂ Catalysts for CO Oxidation ”
S. Deevi, Philip Morris U.S.A., M. Khoudiakov, and M. C. Gupta, Old Dominion University, U.S.A.
- 18:00 - 19:00 **Reception (Anderson Gallery)**
- 20:00 - 21:30 **POSTER SESSION I (Empire Room)**

Tuesday, November 11

SESSION D: QUANTUM DOTS

Chairman: S. Bandyopadhyay

- 8:30 - 8:55 “Electronic Structure of Quantum Dot Lattices”
S. M. Reimann, Lund University, Lund, Sweden
- 8:55 - 9:20 “Quantum Dots and Quantum Dot Arrays: Photogenerated Carrier Relaxation Dynamics, Self-Assembly by Proteins, and Applications to Photon Conversion”
A. J. Nozik, National Renewable Energy Laboratory, Colorado, U.S.A.
- 9:20 - 9:45 “Ab-initio Simulations of Semiconductor Nanostructures”
Giulia Galli, Lawrence Livermore National Laboratory, California, U.S.A.
- 9:45 - 10:00 “Superconducting Coulomb Box as a Switchable Coupling Between Josephson Phase Qubits ”
R. C. Ramos, H. Xu, S. Datta, A. J. Berkley, M. A. Gubrud, F. Strauch, P. R. Johnson, J. R. Anderson, C. J. Lobb, and F. C. Wellstood,
University of Maryland, Maryland, U.S.A.

10:00 - 10:30 **COFFEE BREAK**

SESSION E: NANOWIRES/TUBES

Chairman: A. Baski

- 10:30 - 10:55 “Semiconductor Nanowires and Nanowire Arrays as Smart Sensors”
Martin Moskovits, University of California, Santa Barbara, U.S.A.
- 10:55 - 11:20 “Generation of Diagnostic X-Ray Radiation using a CNT Field Emission Cathode:”
Otto Zhou, University of North Carolina, Chapel Hill, U.S.A.
- 11:20 - 11:45 “Theory of the Electronic, Transport and Optical Properties of Nanotubes”
Steven G. Louie, University of California, Berkeley, U.S.A.
- 11:45 - 12:00 “Semiconductor, Metallic, and Intermetallic Nanoparticle Filaments and Tree-like Assemblies: Synthesis, Properties, and Applications”
V. Abdelsayed and **M. S. El-Shall**, Virginia Commonwealth University,
Richmond, U.S.A.

12:00 - 14:00 **LUNCH BREAK**

SESSION F: NOVEL MAGNETISM

Chairman: A. Arrott

- 14:00 - 14:25 “Magnetic Properties of C₆₀ Polymers”
A. N. Andriotis, Institute of Electronic Structure and Laser, Heraklio, Greece
- 14:25 - 14:50 “The Behaviour of Magnetic Metals Made out of Nanocluster Building Blocks”
Chris Binns, University of Leicester, U.K.
- 14:50 - 15:15 “Ferromagnetic Semiconductor Spintronics Materials and Devices”
Hideo Ohno, Tohoku University, Japan
- 15:15 - 15:30 “Molecular-Scale Spintronics”
R. Pati, L. Senapati, P. M. Ajayan, and **S. K. Nayak**, Rensselaer Polytechnic Institute, New York, U.S.A.
- 15:30 - 16:00 **COFFEE BREAK**

SESSION G: ELECTRICAL AND OPTICAL PROPERTIES

Chairman: H. Morkoç

- 16:00 - 16:25 “Ferroelectricity in Ultra-Cold Free Metal Clusters: A Precursor to Superconductivity”
Walt A. deHeer, Georgia Institute of Technology, U.S.A.
- 16:25 - 16:50 “Plasmonic Nanostructures: Optical Design at Nanoscale Dimensions”
Naomi Halas, Rice University, U.S.A.
- 16:50 - 17:15 “Geometry Driven Interfacial Phenomena in Semiconductor-Metal Hybrid Structures: Extraordinary magnetoresistance and Extraordinary Piezoconductance”
S. A. Solin, Washington University, St. Louis, U.S.A.
- 17:15- 17:30 “Light-Torqued Nanomotors in a Standing Wave”
K. Bonin and A. Shelton, Wake Forest University, Winston-Salem, U.S.A.
- 19:00 **BANQUET**
VIRGINIA MUSEUM OF FINE ARTS

Wednesday, November 12

SESSION H: CLUSTERS ON SUPPORT

Chairman: M. Duncan

- 8:30 - 8:55 “Controlling the Motion of Molecules on the Atomic Scale”
A. J. Heinrich, IBM Almaden Research Center, San Jose, U.S.A.
- 8:55 - 9:20 “Nanoscale Control of Supramolecular Assemblies”
Klaus Kern, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
- 9:20 - 9:45 “Size Controlled Nanostructures by Cluster Deposition: From Softlanding to Implantation”
W. Harbich, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- 9:45 - 10:10 “Nanostructured Surfaces from Size-selected Clusters: From Physics to Biology”
R. E. Palmer, The University of Birmingham, Birmingham, U.K.

10:10 - 10:30 **COFFEE BREAK**

SESSION I: NANO-GROWTH ON STRAINED SURFACES

Chairman: S. Brown

- 10:30 - 10:55 “Self-organized Formation of Nanostructures in Strained Thin Films”
Feng Liu, University of Utah, U.S.A.
- 10:55 - 11:20 “Alignment of Nano-Chains Driven by Cluster Deposition on Constrained Surface”
C. Bréchnac, CNRS Université Orsay Cedex, France
- 11:20 - 11:45 “Order at Soft-Hard Interfaces”
Pulak Dutta, Northwestern University, Evanston, IL, U.S.A.
- 11:45 - 12:00 “Influence of Structural Relaxation on the Optical and Electronic Properties of Ge and Si Nanocrystals”
H.-C. Weissker, J. Fürthmüller, and F. Bechstedt, Friedrich-Schiller-Universität, Jena, Germany

12:00 - 14:00 **LUNCH BREAK**

SESSION J: MULTI-SCALE MODELLING: FROM PHYSICS TO BIOLOGY

Chairman: M. Manninen

- 14:00 - 14:25 “Coulomb Blockade in Gold Nanoclusters”
R. M. Nieminen, Helsinki University of Technology, Espoo, Finland
- 14:25 - 14:50 “Simulation of Chemical Reactions in Enzymes with a Density Function Theory QM/MM Free Energy Method”
Weitao Yang, Duke University, Durham, U.S.A.
- 14:50 - 15:15 “de Novo Computational Chemistry and Applications to Clusters and Nanoassemblies”
William A. Goddard, III, California Institute of Technology, Pasadena, U.S.A.
- 15:15 - 15:30 “Polymer Relaxational Dynamics in Confined Geometry ”
J.-M. Zanotti, M.-L. Saboungi and **D. L. Price**, C.N.R.S., Orleans, France

15:30 - 16:00

COFFEE BREAK

SESSION K: BIOLOGY AT MOLECULAR LEVEL

Chairman: L. A. Bloomfield

- 16:00- 16:25 “Dynamics of Trapped Gas Phase DNA: Fraying and Electron Autodetachment”
Joel H. Parks, Harvard University, Cambridge, U.S.A.
- 16:25 - 16:50 “Theoretical and Experimental Aspects on Trapping and Detection of Single and Few Molecules by using Nanoprobes”
Magnus Willander, Gothenburg University and Chalmers University of Technology, Gothenburg, Sweden
- 16:50 - 17:15 “Nanotechnology, Biotechnology and Complexity Theory: Essential Tools for Engineering Hybrid Biotic-Abiotic Systems”
Carlo Montemagno, University of California, Los Angeles, U.S.A.
- 17:15 - 17:30 “Quantum Mechanical Study of Receptor-Ligand interaction at 5-HT₃ Serotonin Receptors”
S. Baldwin, B. K. Rao, P. Jena, M. Dukat, and R. A. Glennon,
Virginia Commonwealth University, Richmond, Virginia, U.S.A.
- 17:30 - 20:00 **Dinner Break**
- 20:00 - 21:30 **POSTER SESSION II (Empire Room)**

Thursday, November 13

SESSION L: PROTEIN FOLDING/UNFOLDING

Chairman: K. Bonin

- 8:30 - 8:55 “Exploring the Protein Folding Funnel Landscape: Theory Meets Experiments”
Margaret Cheung, University of Maryland, College Park, U.S.A.
- 8:55 - 9:20 “Protein Unfolding: Rigidity Lost”
M. F. Thorpe, Arizona State University, U.S.A.
- 9:20 - 9:35 “Multispectral Fluorescence Imaging of Basal Cell Carcinoma”
M. B. Ericson, C. Berndtsson, B. Stenqvist, A. –M. Wennberg, O. Larko, and **A. Rosén**, Chalmers University of Technology, Sweden
- 9:35 - 9:50 “The Fabrication, Characterization and Performance of Patterned Substrates for Use as Biological Sensors ”
L. Guirl, S. Tripp, D. Inerowicz, S. Howell, F. Regnier, and **R. Reifenberger**, Purdue University, W. Lafayette, U.S.A.

9:50- 10:30 **COFFEE BREAK**

SESSION M: BIOTECHNOLOGY

Chairman: N. Swami

- 10:30 - 10:55 “Nano-Assemblies Shuttled by Motor Proteins”
Viola Vogel, University of Washington, Seattle, U.S.A.
- 10:55 - 11:20 “Optical Manipulation and Fusion of Micro-Containers for Biotechnology”
Kris Helmerson, National Institute of Standards and Technology, Gaithersburg, U.S.A.
- 11:20 - 11:45 “Building an Interface to Biomolecular Processes with Magnetoelectronics”
Jeff M. Byers, Naval Research Laboratory, Washington, U.S.A.
- 11:45 - 12:10 “Tissue Sensor Interfaces”
Alan Rosenbloom, Carnegie Mellon University and University of Pittsburgh, U.S.A.
- 12:10 – 12:25 “Multifunctional Magnetic Nanowires for Biotechnology Applications”
D. H. Reich, C. S. Chen, C. L. Chien, G. J. Meyer, K. Leong, P. C. Searson, and G. Xiao, Johns Hopkins University, Baltimore, U.S.A.

12:25 - 14:00

LUNCH BREAK

14:00 - 16:00

SESSION N: PANEL DISCUSSION

Moderator: R. Compton

Panel Members:

K. H. Bowen - Johns Hopkins University - *Clusters and Cluster Assembled Materials*

G. A. Prinz - Naval Research Laboratory - *Nano Assemblies-Magnetism*

R. S. Berry - University of Chicago - *Theory - Clusters to Proteins*

R. W. Siegel - Rensselaer Polytechnic Institute - *Nano-Structures in Biology*

H. Frauenfelder - Los Alamos National Laboratory - *Physics in Biology*

M. Roco - National Science Foundation - *Nano-Science and Technology : Government Perspective*

16:00

Concluding Remarks - **B. K. Rao**, Virginia Commonwealth University, U.S.A.