Conference Program

Excited State Processes in Electronic and Bio Nano-Materials

October 1-4, 2007
Los Alamos, New Mexico, USA


Sponsored by Center for Nonlinear Studies, Theoretical, Chemistry, Materials Science and Technology, and Bioscience Divisions at Los Alamos National Laboratory and supported by the U.S. Department of Energy.

Scientific Advisors: Alan R. Bishop, Andrew P. Shreve, and Victor I. Klimov

Location: Lodge at Santa Fe (http://hhandr.com/san_main.php), Santa Fe, NM
Monday, October 1

08:00am – 08:40am  Registration
08:40am – 09:00am  Welcome:

**Biosystems/catalysis/molecular aggregates**

*Session chair: James McCusker (Michigan State University)*

09:00am – 09:45am  William Goddard (Caltech)
"New methods for Excited State Processes and applications to nanoelectronic systems"

09:45am – 10:30am  Geoffrey Strouse (Florida State University)
"Nanometal Surface Energy Transfer: Application for Optical Rulers in Biomolecular Processes"

10:30am – 10:45am  Break

10:45am – 11:30am  David Beratan (Duke University)
“Protein electron transfer: when and why does structure matter?”

11:30am – 12:15pm  Mookie Baik (Indiana University)
“Understanding Water Oxidation Catalysis: Insights from Computer Simulations”

12:15pm – 12:35pm  Xinzheng Yang (University of South Carolina)
“Electronic Structure Study of a Novel Series of 2-Dimensional Trimetallic Cluster Complexes, \( \text{Ru}_3(\text{CO})_9(\mu-\text{SnPh}_2)_3[\text{Pt}(\text{PBu}_3)]_x, x = 0 – 3 \)"

12:35pm – 02:00pm  Lunch

*Session chair: Andrew Shreve (LANL)*

02:00pm – 02:45pm  Rienk van Grondelle (Vrije Universiteit, Netherlands)
“The mechanism of photoprotective energy dissipation in higher plants”

02:45pm – 03:30pm  Jasper Knoester (University of Groningen, Netherlands)
“Excitons in molecular aggregates: dynamics, statistics, ensemble and single-molecule spectroscopy”

03:30pm – 03:45pm  Break

03:45pm – 04:30pm  Steven Gray (ANL)
“Theoretical Modeling of Surface Plasmon Excitations in Metallic Nanostructures for Enhanced Nonlinear Responses and Chemical and Biological Sensing”

04:30pm – 05:15pm  David Yaron (Carnegie Mellon University)
“Computational modeling and design of fluorescent dyes for bioimaging”

05:15pm – 05:45pm  Discussion Panel
*Moderators: James McCusker (Michigan State University) and Andrew Shreve (LANL)*

05:30pm  Reception/Cash bar
Tuesday, October 2

Nonlinear optical materials/sensors

Session chair:
08:40am – 09:25am  Uwe Kortshagen (University of Minnesota)
“Plasma synthesis, functionalization, and luminescent properties of silicon nanocrystals”

09:25am – 10:10am  Mireille Blanchard-Desce (University of Rennes, France)
“Molecular to supra molecular engineering for multiphotonics and related applications”

10:10am – 10:55am  Hans Agren (Royal Institute of Technology, Sweden)
“Multiphysics Modeling of Nonlinear Properties: Molecules and Nanoparticles”

10:55am – 11:10am  Break

11:10am – 11:55am  Vladimir Chernyak (Wayne State University)
“Exciton Scattering Approach for Electronic Excitations in Conjugated Molecules: From Oligomers to Organic Networks.”

11:55am – 12:40pm  Rick Averitt (Boston University)
“Terahertz Metamaterial Devices”

12:40pm – 02:00pm  Lunch

Carbon nanotubes

Session chair:  Steven Doorn (LANL)
02:00pm – 02:45pm  Tony Heinz (Columbia University)
“The nature and dynamics of excited states in carbon nanotubes”

02:45pm – 03:30pm  Phaedon Avouris (IBM)
“Photonics and Optoelectronics of Carbon Nanotubes”

03:30pm – 03:45pm  Break

03:45pm – 04:30pm  Larry Luer (Politecnico di Milano, Italy)
“Exciton size and diffusion in (6,5) carbon nanotubes”

04:30pm – 05:15pm  Anne Kelley (UC Merced)
“Surface enhanced resonance Raman scattering and excited state processes on metal nanoparticles”

05:15pm – 05:45pm  Discussion Panel
Moderators:  Steven Gray (ANL)

Poster Session
Poster session chair:  Sergei Tretiak (LANL)
05:45pm – 06:00pm  Preparation
06:00pm – 08:00pm  Poster Session, Reception
Wednesday, October 3

Conjugated polymers/Devices

Session chair: Valy Vardeny (University of Utah)

08:40am – 09:25am  Laurens Siebbeles (TU Delft, Netherlands)  
“Fundamental studies of charge and exciton dynamics in conjugated organic materials”

09:25am – 10:10am  Michael Winokur (University of Wisconsin)  
“How Structure Impacts Optical Properties in Polyfluorene Thin Films”

10:10am – 10:30am  Veaceslav Coropceanu (GaTech)  
“Electron-Phonon Interaction in Organic Molecular Semiconductors”

10:30am – 10:45am  Break

10:45am – 11:30am  Show-An Chen (National Tsing Hua University, Taiwan)  
“Efficient electro-phosphorescence from phosphor-doped conjugated polymers with high and low triplet energies”

11:30am – 12:15pm  John Lupton (University of Utah)  
“How chain conformation controls the photophysics of single conjugated polymer molecules”

12:15pm – 12:35pm  Cungeng Yang (University of Utah)  
“Polaron Spin-lattice Relaxation Time Obtained from Optically Detected Magnetic Resonance Dynamics in π-Conjugated Polymers”

12:35pm – 02:00pm  Lunch

Session chair: Enrique Batista (LANL)

02:00pm – 02:45pm  Gary Rumbles (NREL)  
“Time-resolved Microwave Studies of Conjugated Polymer Bulk Heterojunctions: Advancing Excitonic Solar cells”

02:45pm – 03:30pm  Darryl Smith (LANL)  
“Comparison of spin generation in organic and inorganic semiconductors”

03:30pm – 03:45pm  Break

03:45pm – 04:30pm  Christoph Boehme (University of Utah)  
“Electrical detection of spin coherence in organic devices - how does it work and what can we learn from this?”

04:30pm – 05:15pm  Arkady Yartsev (Lund University, Sweden)  
“Optimal control of barrierless photo-isomerization in cyanines”

05:15pm – 05:45pm  Discussion Panel  
Moderators: Valy Vardeny (University of Utah)

06:30pm  Banquette
Thursday, October 4

Quantum dots/hybrid materials/interfaces/spectroscopy

Session chair:

08:40am – 09:25am  David Nesbitt (JILA)
“Blinking Dynamics in Quantum Dots: Insights from Time Domain and Chemical Studies”

09:25am – 10:10am  Alexander Efros (NRL)
“Mode locking of electron spin coherence in ensemble of charged quantum dots”

10:10am – 10:55am  Philippe Guyot-Sionnest (University of Chicago)
“Switching the luminescence with charged dots and investigations of the Auger mechanism”

10:55am – 11:10am  Break

11:10am – 11:55am  Masaru Kuno (University of Notre Dame)
“Recent perspectives on the optical properties of solution-based nanowires”

11:55am – 12:40pm  Marija Drndic (University of Pennsylvania)
“High-resolution device fabrication for nanocrystal-based electronics and blinking studies”

12:40pm – 02:00pm  Lunch

Session chair:  Andrei Piryatinski (LANL)

02:00pm – 02:45pm  Toni Taylor (LANL)
“TBA”

02:45pm – 03:30pm  Benjamin Schwartz (UCLA)
“TBA”

03:30pm – 03:45pm  Break

03:45pm – 04:30pm  Han Htoon (LANL)
“Polarization-resolved fine structure and magneto-optics of single CdSe nanocrystal quantum dots”

04:30pm – 04:50pm  Randy Ellingson (NREL)
“Multiple Exciton Generation in Colloidal Nanocrystals for Enhanced Solar Energy Conversion”

04:50pm – 05:10pm  Zilvinas Rinkevicius (Institute of Technology, Sweden)
“Second harmonic generation in SiO$_2$/Si(111) interface: density functional theory investigation”

05:10pm – 05:40pm  Discussion Panel
Moderators:  Richard Schaller (LANL)

05:40pm – 05:45pm  Closing Remarks