

Updated 9/11/07

Conference Program

**Excited State Processes in
Electronic and Bio Nano-Materials**

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

<http://cnls.lanl.gov/~esp/esp2007.html>

*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.*

Organizers: Sergei Tretiak, Avadh Saxena, and Richard L. Martin.

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, $Ru_3(CO)_9(\mu-SnPh_2)_3[Pt(PBu^t_3)]_x$, $x = 0 - 3$ "

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 SiO₂/Si(111) interface: density functional theory investigation”

05:10pm – 05:40pm **Discussion Panel**

Moderators:

Richard Schaller (LANL)

05:40pm – 05:45pm **Closing Remarks**