

Updated 8/5/05

Conference Program

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

August 8-11, 2005
Los Alamos, New Mexico, USA

<http://cnls.lanl.gov/~esp/esp2005.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: Hotel Santa Fe (<http://www.hotelsantafe.com>), Santa Fe, NM., NM

Monday, August 8

08:00am – 08:40am **Registration**

08:40am – 09:00am **Welcome:** Alan Bishop (*T-division Director*), Zoltan Toroczkai (*CNLS Deputy Director*), Rod Garcia (*Conference Coordinator, CNLS*)

Biosystems and molecular aggregates

Session chair: Philip J. Hay (LANL)

09:00am – 09:45am **Steven Boxer** (Stanford University)

"Excited state processes reflect chromophore-protein interactions"

09:45am – 10:30am **Stefan Franzen** (North Carolina State University)

"New Materials and Phenomena in Surface Plasmon Resonance Biosensing"

10:30am – 10:45am **Break**

10:45am – 11:30am **Giulio Cerullo** (Politecnico of Milan, Italy)

"Early events of energy relaxation dynamics in carotenoids in solution and inside light-harvesting complexes"

11:30am – 12:15pm **Patrik Callis** (Montana State University)

"QM-MM computation of short range photoinduced electron transfer rates in proteins"

12:15pm – 12:35pm **Philipp Kukura** (UC Berkeley)

"Direct structural observation of the primary isomerization event in vision with femtosecond stimulated Raman"

12:35pm – 02:00pm **Lunch**

Session chair: Andrew Shreve (LANL)

02:00pm – 02:45pm **Todd Martinez** (University of Illinois)

"First Principles Dynamics of Photoisomerization and Photoinduced Proton Transfer"

02:45pm – 03:30pm **Richard B. Dyer** (LANL)

"Protein dynamics in folding and function"

03:30pm – 03:45pm **Break**

03:45pm – 04:30pm **Alex Benderskii** (Wayne State University)

"Dynamics at Surfaces and Interfaces by Spectrally- and Time-Resolved Vibrational Spectroscopy"

04:30pm – 04:50pm **Oleg Poluektov** (Argonne National Laboratory)

"Tuning of Protein Structure in Response to Charge Separation in Photosynthetic Reaction Centers: Time-Resolved High-Field ENDOR of the Spin-Correlated Radical Pair P865⁺QA⁻."

04:50pm – 05:20pm **Discussion Panel**

Moderators: Anne Myers Kelley (UC Merced) and David Nesbitt (U. Colorado)

05:30pm **Reception/Cash bar**

Tuesday, August 9

Transition metals/(bio)sensors/solar cells

Session chair: Richard Averitt (LANL)

09:00am – 09:45am James McCusker (MSU)

“Hot Injection and Chromophore Design in Transition Metal-based Dye-Sensitized Solar Cells”

09:45am – 10:30am Antonin Vlcek (University of London, United Kingdom)

“Ultrafast Excited State Processes of Organometallics: From Excitation to Photochemistry”

10:30am – 10:45am Break

10:45am – 11:30am Daniel Nocera (MIT)

“Microlasers for High Gain Chemosensing ”

11:30am – 12:15pm Antoni Llobet (University of Barcelona, Spain)

“New Ru complexes as functional models for the oxygen evolving center of green plants photosystem II ”

12:15pm – 12:35pm Enrique Batista (LANL)

“Exciton localization in Pt-acetylide complexes”

12:35pm – 02:00pm Lunch

Session chair: Jeanne Robinson (LANL)

02:00pm – 02:45pm David Morris (LANL)

“Molecular Excited States in Organo-f-Element Complexes: Evidence for Vibronic Coupling at the Bottom of the Periodic Table”

02:45pm – 03:30pm Mohammad Omary (University of North Texas)

“Custom-making Phosphors for Solid-State Lighting via Photoinduced Jahn-Teller Distortions, Heavy-atom Effect, and Energy Transfer”

03:30pm – 03:45pm Break

03:45pm – 04:30pm Susan Dexheimer (Washington State University)

“Ultrafast dynamics of localization: quasi-one-dimensional molecular solids and disordered semiconductors”

04:30pm – 04:50pm Veaceslav Coropceanu (Georgia Institute of Technology)

“The roles of vibronic and electronic couplings in organic mixed-valence compounds”

04:50pm – 05:20pm Discussion Panel

Moderators: Thomas Meyer (University of North Carolina) and Richard Martin (LANL)

Poster Session

Poster session chair: Sergei Tretiak (LANL)

05:20pm – 05:45pm Preparation

05:45pm – 08:00pm Poster Session, Reception

Wednesday, August 10

Quantum dots/hybrid materials/interfaces

Session chair: Darryl Smith (LANL)

09:00am – 09:45am Hedi Mattoussi (NRL)

“Use of quantum dots to design biological assay based on resonance energy transfer”

09:45am – 10:30am Richard Schaller (LANL)

“Direct Measurements of Ultra-Efficient Carrier Multiplication in Semiconductor Quantum Dots”

10:30am – 10:45am Break

10:45am – 11:30am Tadashi Itoh (Osaka University, Japan)

“Biexcitonic Lasing in CuCl Quantum Dots and its Characteristic Mechanism”

11:30am – 12:15pm Sergio Ulloa (Ohio University)

“Polarization and Orientation Effects on Coherent Energy Transfer in Semiconductor Nanocrystals”

12:15pm – 12:35pm Gregory Scholes (University of Toronto)

“Exciton spin flip dynamics in colloidal quantum dots”

12:35pm – 02:00pm Lunch

Session chair: Toni Taylor (LANL)

02:00pm – 02:45pm Paras Prasad (University at Buffalo)

“Role of Excited Processes at the Nano: Bio Interface”

02:45pm – 03:10pm Jennifer Hollingsworth (LANL)

“Surface-Dictated and Surface-Mediated Quantum Dot Photoluminescence and Energy Transfer”

03:10pm – 03:30pm Vasiliy Fomenko (University of Colorado)

“Time dependent fluorescence and blinking in semiconductor quantum dots”

03:30pm – 03:45pm Break

03:45pm – 04:05pm Madalina Furis (LANL)

“Probing Exciton Spin States in CdSe Nanocrystals Using Resonant Photoluminescence”

04:05pm – 04:25pm Eugene Tsiper (NRL)

“On the optical matrix element in tight-binding approximation”

04:25pm – 04:45pm Sergei Ivanov (LANL)

“Exciton wavefunction engineering using heterostructured core/shell semiconductor QDs”

04:45pm – 05:15pm Discussion Panel

Moderators: Alexandr Efros (Naval Research Laboratory) and Victor Klimov (LANL)

06:00pm Banquette

Thursday, August 11

Carbon nanotubes/conjugated polymers

- Session chair:* Brian Crone (LANL)
- 09:00am – 09:45am** **Guglielmo Lanzani** (Politecnico of Milan, Italy)
“Real time observation of nonlinear vibrational mode coupling in carbon nanotubes”
- 09:45am – 10:30am** **John Papanikolas** (University of North Carolina)
“Ultrafast Dynamics in Single-Walled Carbon Nanotube (SWNT)/Polymer Composites”
- 10:30am – 10:45am** **Break**
- 10:45am – 11:30am** **Zeev Valy Vardeny** (University of Utah)
“Ultrafast exciton dynamics in single-walled nanotubes”
- 11:30am – 12:15pm** **Steve Doorn** (LANL)
“Raman Studies of Single Walled Carbon Nanotubes”
- 12:15pm – 12:35pm** **Valeria Kleiman** (University of Florida)
“Vectorial Energy transfer in phenyl ethynylene dendrimers”
- 12:35pm – 02:00pm** **Lunch**
- Session chair:* Shawn McGrane (LANL)
- 02:00pm – 02:45pm** **Adrian Roitberg** (University of Florida)
“Influence of structure and dynamics on energy transfer rates in dendrimers”
- 02:45pm – 03:30pm** **Peter Weber** (Brown University)
“Characterization of molecular shape and charge distributions by Rydberg fingerprint Spectroscopy”
- 03:30pm – 03:45pm** **Break**
- 03:45pm – 04:30pm** **Glenn Bartholomew** (University of Washington)
“Synthesis and Photophysics of Carbohydrate-Derivatized PPV Oligomers in Water”
- 04:30pm – 04:50pm** **Anne Myers Kelley** (UC, Merced)
“Tunable resonance hyper-Raman spectroscopy of nonlinear optical Chromophores”
- 04:50pm – 05:20pm** **Discussion Panel**
Moderators: Gregory Scholes (University of Toronto) and Vladimir Chernyak (Wayne State University)
- 05:20pm – 05:25pm** **Closing Remarks**

Poster Session

Tuesday, August 9

1. Ekaterina Badaeva (New Mexico Highlands)

“Role of donor-acceptor strengths and separation on the two-photon absorption response of cytotoxic dyes: a TD-DFT study”

2. Tom Baker (University of Colorado)

“Scanning Photoionization Microscopy of Thin Metal Films”

3. Marta Cerruti (North Carolina State)

“Thermographic detection of DNA microarrays”

4. Elbert Chia (LANL)

“Time-resolved optical conductivity study of the itinerant antiferromagnet UNiGa5 via pump-probe spectroscopy”

5. Aaron Clapp (NRL)

“Observing simultaneous molecular scale interactions using quantum dots in a FRET-based multiplexing format”

6. Josh Coe (University of Illinois)

“Ab Initio Multiple Spawning Dynamics of Excited State Proton Transfer and Three-State Intersection Dynamics”

7. Mircea Cotlet (LANL)

“Single molecule spectroscopic characterization of a far red fluorescent protein (HcRed) from the Anthozoa coral Heteractis crispa”

8. Veaceslav Coropceanu (Georgia Institute of Technology)

“The roles of vibronic and electronic couplings in organic mixed-valence compounds.”

9. Cristian Diaconu (LANL)

“Charge carrier mobilities in wires and films of oligoacenes from hybrid density functional calculations”

10. Tienneke Dykstra (University of Toronto)

“Time-Evolution of Excitations in a Conformationally Disordered Conjugated Polymer”

11. Demetrio Filho (Georgia Institute of Technology)

“Semiempirical and ab initio calculation of transfer integrals: Application to p-type and n-type Organic semiconductors”

- 12. Serge Gorelsky** (Stanford University)
"Spectroscopic and DFT Investigation of $[M\{HB(3,5-iPr_2pz)_3\}(SC_6F_5)]$ ($M = Mn, Fe, Co, Ni, Cu, \text{ and } Zn$) Model Complexes: Periodic Trends in Metal-Thiolate Bonding"
- 13. Serguei Goupalov** (LANL)
"Chirality dependence of the Raman cross-section of carbon nanotubes"
- 14. Sean Hightower** (University of Wyoming)
*"The Nature of the Lowest Excited States of Cp^*TaCl_4 and Related Complexes: "Mixed-up" Molecules that Change Orbital Character Upon Ligand Variation"*
- Sean Hightower**
- 15. Joshua Kennedy** (University of Utah)
"Electroabsorption spectroscopy of single-walled carbon nanotubes"
- 16. Dmitri Kilin** (University of Washington)
"Nonadiabatic dynamics of photoexcitation in nanoparticle-organic molecule heterocomposites"
- 17. Svetlana Kilina** (University of Washington)
"Excitonic and vibrational effects in carbon nanotubes"
- 18. Oleg Korovyanko** (Argonne National Laboratory)
"Ultrafast Charge Generation and Detection in Organic Electronic Materials Using High-Energy Electron Excitations"
- 19. Philipp Kukura** (UC Berkeley)
"Direct structural observation of the primary isomerization event in vision with femtosecond stimulated Raman"
- 20. Youmei Lu** (New Mexico Highlands)
"Effect of photosensitivity from the terminal group in two-photon induced processes"
- 21. Artem Masunov** (University of Central Florida)
"Theoretical study of solvent effects on electronic structure and spectra of paracyclophane chromophores"
- 22. Serguei Pachtchenko** (Argonne National Laboratory)
"Bidirectional Electron Transfer in Photosystem I: Direct Evidence from High-Frequency Time-Resolved EPR"
- 23. Yuriy Pereverzev** (University of Washington)
"Dissipation of classical energy in nonlinear quantum systems"
- 24. Andrei Piryatinski** (LANL)
"Semiclassical Scattering on Conical Intersections"

- 25. Sergei Ponomarev** (Wesleyan University)
"Ion motions in molecular dynamics simulations on DNA"
- 26. Crissy Rhodes** (North Carolina State)
"SPR on Conducting Metal Oxides"
- 27. Ilya Rumyantsev** (University of Toronto)
"All-optical AC Spin Currents via Excitonic Quantum Interface"
- 28. Chuanxiang Sheng** (University of Utah)
"Ultrafast photogenerated excitons, polarons, and solitons in trans-polyacetylene"
- 29. Minghong Tong** (University of Utah)
"Superfluorescence in distyryl-benzene single crystals"
- 30. Ping Yang** (Michigan Technological University)
"First principle study of surface ligand binding to small CdSe clusters"