

Program

Excited State Processes in Electronic and Bio-Materials

August 13-16, 2001
Los Alamos, New Mexico, USA

Sponsored by Center for Nonlinear Studies, Theoretical, Chemistry, 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, Robert J. Donohoe, and Victor Klimov

Location: Conference Room, Los Alamos Inn, 2201 Trinity Drive, Los Alamos, NM

Monday, August 13

08:30am – 09:40am **Registration**

09:40am – 09:50am **Welcome**

Dr. Len Margolin (*Deputy Director, CNLS*)

Dr. Carol J. Burns (*Deputy Director, Chemistry Division*)

Rod Garcia (*Conference Coordinator, CNLS*)

Biological Systems and Molecular Aggregates

Session chair: Dr. Benjamin H. McMahon (LANL)

09:50am – 10:40am **Prof. Klaus Schulten** (the University of Illinois)

“Excitons in a photosynthetic light-harvesting system: a combined molecular dynamics/quantum chemistry, polaron model, and random matrix study”

10:40am – 11:30am **Prof. Gerald J. Small** (Iowa State University)

“Spectral hole burning with high pressure and external electric fields: probing interactions in strongly coupled aggregates”

11:30am – 11:45am **Coffee Break**

11:45am – 12:35am **Prof. Shaul Mukamel** (the University of Rochester)

“Multidimensional spectroscopy of molecular aggregates and peptides: femtosecond snapshots of electronic and vibrational coherence”

12:35pm – 02:00pm **Lunch**

Session chair: Dr. Angel E. García (LANL)

02:00pm – 02:50pm **Dr. Andrew P. Shreve** (LANL)

“Exploration of excited electronic and vibrational states in molecular charge transfer solid state materials”

02:50pm – 03:40pm **Prof. Todd J. Martinez** (the University of Illinois)

“First principles simulation of photoinduced cis-trans isomerization”

03:40pm – 03:55pm **Coffee Break**

03:55pm – 04:45pm **Dr. William H. Woodruff** (LANL)

“Dynamics of oxidase enzymes from picoseconds to kiloseconds”

04:45pm – 05:35pm **Discussion Panel**

Moderators: Prof. Gerald J. Small, Prof. Shaul Mukamel

06:00pm **Reception**

Tuesday, August 14

Electronic Interactions in Semiconductor Quantum Dots

- Session chair:* Dr. Antoinette J. Taylor (LANL)
- 09:00am – 09:50am Prof. Philippe Guyot-Sionnest** (the University of Chicago)
“n-type semiconductor nanocrystal colloids, intraband spectroscopy and dynamics”
- 09:50am – 10:40am Dr. Victor I. Klimov** (LANL)
“Semiconductor quantum dots: From fundamental physics to optical devices”
- 10:40am – 10:55am Coffee Break**
- 10:55am – 11:45am Prof. Mostafa A. El-Sayed** (Georgia Inst. of Technology)
“Shape dependent properties of semi-conductor nanocrystals”
- 11:45am – 12:10pm Dr. Alexandre A Mikhailovski** (LANL)
“Electron and hole intra-band dynamics in nanocrystal quantum dots”
- 12:10pm – 12:35pm Christy Landes** (Georgia Inst. of Technology)
“Changes in the opto-electronic properties of CdSe nanoparticles as their size approaches 1.0 nm”
- 12:35pm – 02:00pm Lunch**
- Session chair:* Dr. Jennifer Hollingsworth (LANL)
- 02:00pm – 02:50pm Prof. Mounqi G. Bawendi** (MIT)
“Semiconductor nanocrystals: single dots, charged dots, lasing dots”
- 02:50pm – 03:40pm Dr. Scott A. Crooker** (LANL)
“Spins in quantum dots: Optical spectroscopy to 60 Tesla”
- 03:40pm – 03:55pm Coffee Break**
- 03:55pm – 04:45pm Discussion Panel**
Moderators: Prof. Mounqi G. Bawendi, Dr. Victor I. Klimov
- 06:30pm Banquette**

Wednesday, August 15

Excited State Potentials and Ultrafast Processes

- Session chair:* Dr. Edward M. Kober (LANL)
- 09:00am – 09:50am** Prof. Jean-Luc Bredas (the University of Arizona)
“Characterization of the charge transfer and transport processes in semiconducting polymers and molecular crystals”
- 09:50am – 10:40am** Prof. Anne B. Myers-Kelley (KSU)
“Solvent and aggregation effects on ground and excited-state structures of nonlinear push-pull chromophores”
- 10:40am – 10:55am** Coffee Break
- 10:55am – 11:45am** Prof. Guillermo C. Bazan (UCSB)
“Strategies for optimizing interchromophore contacts”
- 11:45am – 12:10pm** Dr. Oleg Korovyanko (the University of Utah)
“Photoexcited states in self-organized polymer solid films”
- 12:10pm – 12:35pm** Glenn Bartholomew (UCSB)
“Paracyclophane-based NLO chromophores: 3D intramolecular charge transfer”
- 12:35pm – 02:00pm** Lunch
- Session chair:* Dr. Duncan W. McBranch (QTL Biosystems)
- 02:00pm – 02:50pm** Dr. Sergei Tretiak (LANL)
“Time-dependent photoexcitation dynamics of conjugated molecules”
- 02:50pm – 03:40pm** Prof. Valy Vardeny (the University of Utah)
“Random lasers in π -conjugated polymer films”
- 03:40pm – 03:55pm** Coffee Break
- 03:55pm – 04:20pm** Andrew Moran (KSU)
“A molecular dynamics study of 3 nonlinear push-pull chromophores”
- 04:20pm – 04:45pm** Dr. Jason McNeill (the University of Texas)
“Imaging carrier generation, recombination, and drift in a conjugated polymer”
- 04:45pm – 05:10pm** Geoff Hutchison (Northwestern University)
“Electronic structure studies of optics and transport in conjugated polymers”
- 05:10pm – 05:50pm** Discussion Panel
Moderators: Prof. Valy Vardeny, Dr. Duncan W. McBranch
- 06:00pm** Reception

Thursday, August 16

Excited State Potentials and Ultrafast Processes

Session chair: Dr. Jeffrey P. Hay (LANL)

09:00am – 09:50am Prof. Paul F. Barbara (the University of Texas)

“Single molecule spectroscopy of conjugated polymers”

09:50am – 10:40am Prof. Mireille Blanchard-Desce (Univ. de Rennes, France)

“Molecular chromophores for nonlinear optical imaging of biological membranes”

10:40am – 10:55am Coffee Break

10:55am – 11:45am Prof. Sumit Mazumdar (the University of Arizona)

“Electron correlations and light emission in conjugated polymers and oligomers”

11:45am – 12:10pm Dr. Markus Wohlgenannt (the University of Utah)

“Direct determination of singlet and triplet exciton cross-sections for charge recombination in π -conjugated polymers”

12:10pm – 12:35pm Dr. Ilya Bezel (UC, Berkeley)

“Molecular dynamics at metal surface in presence of image-state electron: solvation, polaron formation”

12:35pm – 02:00pm Lunch

Session chair: Dr. Avadh Saxena (LANL)

02:00pm – 02:50pm Prof. David Yaron (Carnegie Mellon University)

“New approaches to quantum chemical calculations on conjugated polymers: from band theory to disordered systems”

02:50pm – 03:15pm Dr. Darryl L. Smith (LANL)

“Excitation transfer processes in a phosphor doped light emitting diodes”

03:15pm – 03:40pm Dr. Jon R Schoonover (LANL)

“Recent applications of transient infrared spectroscopy in a study of excited states in metal polypyridyl complexes”

03:40pm – 04:05pm Dr. Richard L. Martin (LANL)

“Analyzing the transition density: a compact orbital representation”

04:05pm – 04:15pm Closing remarks

Dr. Alan R. Bishop (*Theoretical Division Director*)