Updated 8/7/03

Conference Program

Excited State Processes in Electronic and Bio Nano-Materials

August 11-16, 2003
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.

Organizers: Sergei Tretiak, Avadh Saxena, and Richard L. Martin.
Scientific Advisors: Alan R. Bishop, Andrew P. Shreve, and Victor I. Klimov

Location: Motorola Building, Los Alamos Research Park, Los Alamos, NM

Monday, August 11

08:00am – 08:30am **Registration**
08:30am – 08:55am **Welcome:** Don Parkin *(CINT Associate Director, MST Division)***,** Rod Garcia *(Conference Coordinator, CNLS)*

Biological Systems and Molecular Aggregates

Session chair: Todd Martinez (University of Illinois)

08:55am – 09:40am **Paul Champion** (Northeastern University)
"Exploring low frequency modes in biomolecules using femtosecond coherence spectroscopy"

09:40am – 10:25am **Alexei Stuchebrukhov** (University of California, Davis)
"Electron transfer in proteins"

10:25am – 10:40am **Break**

10:40am – 11:25am **Shigehiko Hayashi** (Kyoto University, Japan)
"Molecular dynamics simulation of bacteriorhodopsin's photoisomerization using ab initio forces for the excited chromophore"

11:25am – 12:10pm **Sharon Hammes-Schiffer** (Pennsylvania State University)
"Proton-coupled electron transfer reactions"

12:10pm – 12:35pm **Yang Zhao,** M-F. Ng, and G. Chen (University of Hong Kong)
"Low-lying excited states of light-harvesting system II in purple bacteria"

12:35pm – 02:00pm **Lunch**

Session chair: Darryl Smith (LANL)

02:00pm – 02:45pm **Qiang Cui** (University of Wisconsin, Madison)
"Molecular simulations of mechanochemical coupling in molecular motors"

02:45pm – 03:30pm **GuanHua Chen** (University of Hong Kong, Hong Kong)
"Optical response and field emission of carbon nanotubess"

03:30pm – 03:55pm **Verner Kristian Thorsmølle** (LANL)
"Ultrafast conductivity dynamics in pentacene probed using terahertz time-domain spectroscopy"

03:55pm – 04:10pm **Break**

04:10pm – 04:55pm **Marilu' Ariu** (University of Sheffield, UK)
"Energy transfer and light emission in organic semiconductors"

04:55pm – 05:40pm **David Beljonne** (Université de Mons, Belgium)
"Quantum-chemical modeling of charge and energy transfer in supramolecular assemblies"

05:40pm – 06:00pm **Discussion Panel**
Moderator: David Yaron and Todd Martinez

06:00pm **Reception**

Tuesday, August 12

Biological Systems and Molecular Aggregates

Session chair: David Yaron (Carnegie Mellon University)

08:30am – 09:15am **Devens Gust** (Arizona State University)
"Molecular photovoltaics, switches, and photonic wires based on porphyrins and fullerenes"

09:15am – 10:00am **Frank Spano** (Temple University)
"Understanding the photophysical properties of lamellar and herringbone aggregates of conjugated oligomers: excitons, phonons and defects"

10:00am – 10:25am **Eugene Tsiper** (Rutgers University)
"Atomic multipole representation of molecular response to external fields"

10:25am – 10:40am **Break**

10:40am – 11:25am **John McKelvey** (McKelvey Computational Chemistry)
"An efficient scheme for determining light absorption properties"

11:25am – 12:10pm **Christopher Bardeen** (University of Illinois)
"Picosecond dynamics in nanoscale aggregates of conjugated organic materials"

12:10pm – 12:35pm **Valter Zazubovich,** R. Jankowiak, K. Riley, M. Rätsep and G. J. Small (Iowa State University) *"Dispersive kinetics of primary charge separation in the isolated reaction center of photosystem II studied with spectral hole burning"*

12:35pm – 02:00pm **Lunch**

Session chair: Alexandr Efros (Naval Research Laboratory)

Semiconductor Quantum Dots

02:00pm – 02:45pm **David Nesbitt** (University of Colorado)
"Time dependent power law fluorescence dynamics semiconductor quantum dots"

02:45pm – 03:30pm **Gregory Scholes** (University of Toronto)
"Relating electronic structure to optical response: comparison of conjugated polymers to semiconductor quantum dots"

03:30pm – 03:45pm **Break**

03:45pm – 04:30pm **David Norris** (University of Minnesota)
"In Vivo Imaging of Quantum Dots"

04:30pm – 04:55pm **Brian Wehrenberg** and P. Guyot-Sionnest (University of Chicago)
"Optical and electrochromic properties of colloidal PbSe nanocrystals"

04:55pm – 05:20pm **Melissa Petruska,** A. V. Malko, P. M. Voyles, and V. I. Klimov (LANL)
"From individual nanocrystals to functional nanocrystal assemblies"

Poster Session

Poster session chair: Sergei Tretiak (LANL)

05:20pm – 06:00pm **Preparation**

06:00pm – 08:00pm **Poster Session, Reception**

Wednesday, August 13

Semiconductor Quantum Dots

Session chair: Victor Klimov (LANL)

08:30am – 09:15am **Arthur Nozik** (NREL)
"Relaxation dynamics and interparticle electron transfer dynamics in photoexcited semiconductor nanocrystals"

09:15am – 10:00am **Alexandr Efros** (Naval Research Laboratory)
"General boundary conditions and effect of the surface on the energy spectra of nanocrystrals"

10:00am – 10:25am **Marc Achermann,** M.A. Petruska, J. A. Hollingsworth, and V. I. Klimov, (LANL) *"Exciton-exciton interactions in semiconductor nanocrystals: The effect on lasing and light harvesting performance"*

10:25am – 10:40am **Break**

10:40am – 11:25am **David Gershoni** (Technion, Israel)
"Semiconductor Quantum dots as sources of correlated multicolor single photons"

11:25am – 12:10pm **David Kelley** (University of California, Merced)
"Electronic spectroscopy of GaSe nanoparticles"

12:10pm – 12:35pm **Richard Schaller**, M. A. Petruska, S. Jeong, J. A. Hollingsworth and V. I. Klimov, (LANL) *"PbSe quantum dots and quantum rods: From optical gain to polarized emission"*

12:35pm – 02:00pm **Lunch**

Session chair: Avadh Saxena (LANL)

02:00pm – 02:45pm **Ananth Dodabalapur** (University of Texas at Austin)
"What can we do with organic transistors?"

02:45pm – 03:10pm **Discussion Panel**
Moderators: Victor Klimov and Alexandr Efros

07:00pm **Banquette**

Thursday, August 14

Semiconductor Quantum Dots

Session chair: Richard Martin (LANL)

08:30am – 09:15am **Todd Krauss** (University of Rochester)
"Localized charge properties of single semiconductor quantum rods"

09:15am – 09:40am **Vanessa Huxter,** M.R. Salvador, and G.D. Scholes (University of Toronto)
"Two dimensional photon echo studies of nanocrystalline quantum dots"

09:40am – 10:05am **Han Htoon,** J. A. Hollingsworth, A. V. Malko, R. Dickerson, and V. I. Klimov (LANL) *"Zero-to-one dimensional transition and Auger recombination in semiconductor nanorods"*

10:05am – 10:20am **Break**

Metal Nanoparticles and Complexes

10:20am – 11:05am **Thomas Meyer** (LANL)
"Photoinduced electron and energy transfer in molecular assemblies"

11:05am – 11:50am **James Brozik** (University of New Mexico)
"Extent of localization in the excited states of platinum acetlynic compounds"

11:50am – 12:15pm **Jiang Jiang** and Louis Brus (Columbia University)
"Single molecule raman spectroscopy at the junctions of large Ag nanocrystals"

12:15pm – 12:40pm **Alexander Mikhailovsky,** J. Ostrowski, M. Katiyar, and G. Bazan (UCSB*) "Control of radiative processes using surface plasmon resonances in metal nanostructures"*

12:40pm – 02:00pm **Lunch**

Session chair: Guillermo Bazan (UCSB)

02:00pm – 02:45pm **Neil Greenham** (Cavendish Laboratory, UK)
"Recombination in polymer heterojunction devices"

02:45pm – 03:30pm **Darryl Smith** (LANL)
"Electron spin injection from ferromagnetic contacts"

03:30pm – 03:45pm **Break**

Organic Electronic Materials and Polymers

03:45pm – 04:30pm **Joseph Perry** (University of Arizona)
"Two-Photon properties of conjugated organic molecules and nanocomposites"

04:30pm – 04:55pm **Egbert Zojer,** D. Beljonne, W. Wenseleers, S.J.K. Pond, M. Rumi, M. Halik, S. Barlow, C. Grasso, J.W. Perry, S. Marder, and J.-L. Brédas (University of Arizona)
"Design of materials with enhanced two-photon absorption properties – influence of ground-state polarization, charge-transfer distance and nature of the conjugated backbone"

04:55pm – 05:20pm **Mariacristina Rumi,** S.J.K. Pond, D.Beljonne, O. Kwon, E. Zojer, M.L. Levin, T.C. Parker, O. Tsutsumi, J.-L. Brédas, S.R. Marder, and J.W. Perry (University of Arizona)
"Substituent effects on the spectroscopic properties of two-photon absorbing chromophores"

05:20pm – 05:45pm **Artem Masunov** and S. Tretiak (LANL)
"Prediction of two photon absorption properties for large organic molecules using time-dependent density functional theory"

05:45pm – 06:10pm **Discussion Panel**

Moderators: Anne Myers Kelley and Guillermo Bazan

Friday, August 15

Organic Electronic Materials and Polymers

Session chair: Zeev Valy Vardeny (University of Utah)

08:30am – 09:15am **Takayoshi Kobayashi** (University of Tokyo, Japan)
"Geometrical relaxation studied by ultrashort pulselaser"

09:15am – 10:00am **Josef Klafter** (Tel Aviv University, Israel)
"Fractional kinetics in transport and relaxation"

10:00am – 10:25am **Andrei Piryatinski,** S. Tretiak, A. Saxena, R.L. Martin, and A.R. Bishop (LANL) *"Non-adiabatic dynamics in electron phonon coupled system"*

10:25am – 10:40am **Break**

10:40am – 11:25am **Alan Bishop** (LANL)
"Photoexcitation and energy localization in soft electronic matter"

11:25am – 12:10pm **Robert Austin** (Princeton University)
"Picosecond conformational dynamics of proteins: proteins are nanomachines in nanotime"

12:10pm – 12:35pm **Vladimir Butko** (LANL)
"Progress in organic single crystal electronics"

12:35pm – 02:00pm **Lunch**

Session chair: Sumit Mazumdar (University of Arizona)

02:00pm – 02:45pm **Kieron Burke** (Rutgers University)
"Time-dependent density functional theory for electronic and bio nanomaterials"

02:45pm – 03:30pm **Vladimir Chernyak** (Corning Inc.)
"Density Functional Theory with Finite Number of Single-Electron Orbitals"

03:30pm – 03:55pm **Ignacio Franco** (University of Toronto) and S. Tretiak (LANL)
"Electron-vibrational dynamics of photoexcited polyfluorenes"

03:55pm – 04:10pm **Break**

04:10pm – 04:55pm **Anna Krylov** (University of Southern California)
"Tuning molecular properties by electronic excitations"

04:55pm – 05:40pm **Filipp Furche** (Universität Karlsruhe, Germany)
"Exploring excited potential energy surfaces by analytical TDDFT derivative methods"

05:40pm – 06:00pm **Discussion Panel**
Moderators: Zeev Valy Vardeny and Sumit Mazumdar

06:00pm **Reception**

Saturday, August 16

Organic Electronic Materials and Polymers

Session chair: Anne Myers Kelley (University of California, Merced)

08:30am – 09:15am **Martin Kirk** (University of New Mexico)
"Low-Dimensional materials: new paradigms for molecular bistability"

09:15am – 09:40am **Rudolph Magyar,** E.K.U. Gross, and A. Fleszar (Rutgers University)
"Exact-exchange density-functional calculations on noble-gas solids"

09:40am – 10:05am **Oleg Korovyanko,** C.-X. Sheng and Z.V. Vardeny, A. Dalton and R. Baughman (University of Utah) *"Ultrafast Photoresponse of Excitons in Single-Walled Carbon Nanotubes"*

10:05am – 10:20am **Break**

10:20am – 10:45am **Geoff Hutchison** (Northwestern University)
"Studies on transparent conducting polymers"

10:45am – 11:10am **Reginaldo Rocha,** M.G. Brown, C.H. Londergan, C.P. Kubiak and A.P. Shreve (LANL) *"Probing mixed-valency in molecular charge-transfer systems"*

11:10am – 11:35pm **Dmitri Kilin,** Y.V. Pereversev, O.V. Prezhdo (University of Washington)
"Electron-nuclear correlations for photoinduced dynamics in molecular dimers"

11:35pm – 12:00pm **Paul Day,** K.A. Nguyen and R. Pachter (WPAFB)
"Theoretical predictions of two-photon absorption in substituted stilbenes: a time-dependent density functional theory study"

12:00pm – 12:15pm **Closing remarks**

Poster Session

Tuesday, August 12

1. Darius Abramavicius and S. Mukamel (University of Rochester)
"Disentangling complex multidimensional spectra of excitons using coherent control"

2. Dmitri Babikov (LANL)
"Quantum Origin of Anomalous Isotope Effect in Ozone Formation"

3. Thomas Baker (JILA and University of Colorado)
"Using Visible Light to Generate Silver Nanoparticles"

4. Andrew Bartko, A. Mikhailovsky, M. Achermann, M.A. Petruska, M.I. Stockman, and V.I. Klimov (LANL)
"Control of Radiative Processes Using Surface Plasmon Resonances in Metal Nanostructures"

5. Enrique Batista (LANL)
"Excited State Calculations of the States Involved in the Luminescent Probe $[Ru(bpy)^2\ dppz]^{2+}$"

6. Liu Bin, G. Bazan, B. Koehler, H. Benmansour, A. Mikhailovsky, and J. Hong (UCSB)
"Two Photon Absorbing Dyes"

7. Joshua Coe (University of Illinois)
"Nonadiabatic Molecular Dynamics in Small Molecules"

8. Nikolai Fomin, E. O. Danilov, A. J. Rodgers, D. L. Snavely (Bowling Green State University)
"Nonlinear Optical Properties of Organic Chromophores Immobilized in Sol-Gel Glasses"

9. Rene Gaudoin (Rutgers University)
"A direct approach to excited states in density functional theory"

10. Kirill Igumenshchev (University of Rochester) and S. Tretiak (LANL) *"Delocalization of photoexcitations in conjugated polymers: a time-dependent density functional theory study"*

11. Hose Hodak, C. Downey, A. Pardi, D. J. Nesbitt (JILA and University of Colorado)
"Single Molecule Folding Dynamics of Ribozyme Construct Fragments"

12. Dmitri Kilin (University of Washington)
"Peak shift modulation for photon echo in molecular dimers"

13. Chaehyuk Ko, B. Levine, and T. J. Martínez (University of Illinois)
"Ab Initio Multiple Spawning Dynamics of the Photoactive Yellow Protein Chromophore"

14. George Kalosakas and I. Bezel (LANL)
"Electron dynamics in low-dimensional organics: intraband relaxation and polaron formation"

15. Nadya Kobko (City University of NY), A. Masunov, S. Tretiak (LANL)
"Study of nonlinear optical response in substituted stilbenes with the time-dependent density functional theory"

16. Weinan Leng and A. Myers Kelley (University of California, Merced)
"Resonance Raman study of interchromophore coupling in monomeric and dimeric merocyanine dyes"

17. Sergey Levchenko and A. I. Krylov (University of Southern California)
"Why electronic states of the three didehydrotoluene isomers are so different? Understanding excited states in open-shell systems by Spin-Flip EOM-CCSD calculations."

18. James Murphy, O. Micic, M. Hanna, R. Ellingson and A. Nozik (NREL and University of Colorado)
"Interdot Electronic Coupling in Quantum Dot Arrays observed using Time-Resolved Terahertz Spectroscopy"

19. Hiromi Nakai, J. Heyd, and G. E. Scuseria (Rice University and Waseda University, Japan)
"Theoretical study of the band structure of rutile and anatase titanium dioxide"

20. Ted Ortiz (University of New Mexico)
"TBA"

21. Denise Pauler and B. Kendrick (LANL)
"Quantum Hydrodynamic Study of Two-Dimensional Reactive Scattering"

22. Juan Peralta and G. E. Scuseria (Rice University)
"Relativistic self-consistent field all-electron calculations including the spin-orbit interaction"

23. Andrei Piryatinski, S. Tretiak, H. Htoon, and V. I. Klimov (LANL) *"Multiparticle Electronic Dynamics in Transition from Zero to One Dimension in Semiconductor Nanostructures"*

24. Garry Rumbles (NREL)
"Quantum Dot Molecules Assembled with Genetically Engineered Proteins"

25. Karin Schmidt (University of Arizona) *"Quantum confinement in quasi-one-dimensional solids with strong coupling of Frenkel and Charge Transfer excitons"*

26. Chuanxiang Sheng, O.J. Korovyanko, Z.V. Vardeny (University of Utah), A.B. Dalton and R.H. Baughman (UT, Dallas)
"Excited-state Relaxation and Photoinduced Dichroism in Single-wall Carbon Nanotubes"

27. Igor Stiopkin, T. Brixner, M. Yang and G. R. Fleming (University of California, Berkeley)
"2D Electronic Spectroscopy of J-aggregates: Theory and Experiment"

28. Eugene Tsiper (Rutgers University)
"Generalized Lanczos method for lowest-frequency excitations in dynamic mean-field calculations"

29. Nina Verdal and A. Myers Kelley (University of California, Merced)
"Coupling of amorphous matrix phonons to the electronic transitions of rigid chromophores"

30. Dmitri Voronine (Bowling Green State University)
"Excited State Dynamics of Mesoscopic Chromophore Aggregates; Dependence on Aggregate Shape"

31. Yongguo Yan, S. Mazumdar, S. Dallakyan, and M. Chandross (University of Arizona)
"Designing π-conjugated polymers with light emission in the infrared"

32. Pingrong Yu, O. Micic, J. Nedeljkovic, R. Ellingson and A. Nozik (NREL and University of Colorado)
"Carrier Cooling Dynamics and Charge Transfer in Semiconductor Nanorods"

33. Wei Zhuang, A. Moran, T. Jansen, and Shaul Mukamel (University of Rochester)
"Two dimensional vibrational snapshots of peptide relaxation triggered by photoisomerization: MD simulation"