January 4, 2008

Sergei Tretiak

Theoretical Division, Mail Stop B268,
Los Alamos National Laboratory
Los Alamos, NM 87545
Phone: (505) 667-8351
Fax: (505) 665-3909
E-mail: serg@lanl.gov
Web: http://www.t12.lanl.gov/home/serg

Personal information

Citizenship:	Russia
Status in the USA:	Permanent Resident
Marital Status:	Married with two children

Education

November 1998	Ph.D. in Chemistry Department of Chemistry, University of Rochester Thesis *"Collective Electronic Excitations in Spectroscopy of Conjugated and Aggregated Molecules"* Supervised by Prof. S. Mukamel
April 1996	M.S. in Chemistry Department of Chemistry, University of Rochester Supervised by Prof. S. Mukamel
April 1994	M.S. in Physics Russian Academy of Sciences, Institute of Spectroscopy Supervised by Prof. E. A. Ryabov
April 1992	B.S. in Physics Department of Problems of Physics and Energetics, Moscow Institute of Physics and Technology

Research Interests

Relation between optical and chemical properties of organic and semiconductor materials; Development of modern computational methods for molecular optical properties; time-dependent density functional theory and semiempirical methods; Nonlinear optical response of organic chromophores; Adiabatic and non-adiabatic molecular dynamics of the excited states; Collective electronic excitations and optical response of confined excitons in conjugated polymers, carbon nanotubes, semiconductor nanoparticles, and molecular aggregates; Charge and energy transfer in biological and artificial antenna complexes; Ultrafast nonlinear spectroscopy; Nonlinear dynamics of complex classical and quantum systems.

Professional Experience

October 2005 – Present	Staff Scientist, Center for Integrated Nanotechnologies (CINT) Los Alamos and Sandia National Laboratories, Albuquerque, NM 87185.
March 2001 – Present	Technical Staff Member, Theoretical Chemistry and Molecular Physics T-12 Group of Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545.
October 2006 – January 2007	CNRS invited professor, UMR 6510 (Synthse et Electrosynthse Organiques) Universit de Rennes 1, Campus de Beaulieu, Bt. 10A, 35042 Rennes Cedex, France.
August 1999 – February 2001	LANL Director's Funded Postdoctoral Fellow, Condensed Matter and Statistical Physics T-11 Group of Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545.
December 1998 – July 1999	Postdoctoral Associate Group of Prof. Shaul Mukamel, Department of Chemistry, University of Rochester, Rochester, NY 14627
September 1994 – November 1998	Graduate Student Group of Prof. Shaul Mukamel, Department of Chemistry, University of Rochester, NY 14627
September 1994 – May 1996	Graduate Teaching Assistant Department of Chemistry, University of Rochester, NY 14627
September 1991 – May 1994	Graduate Student Group of Prof. E. A. Ryabov, Institute of Spectroscopy, Troitsk, Russia.
September 1987 – May 1991	Undergraduate Student Department of Problems of Physics and Energetics, Moscow Institute of Physics and Technology, Dolgoprudny, Russia.

Honors, Fellowships

- ⋆ Slansky Fellow Award [2001], Los Alamos National Laboratory.
- ⋆ LANL Director's Post-Doctoral Fellowship [1999-2001], Los Alamos National Laboratory.
- ⋆ Arnold Weissberger Graduate Fellowship [1997-1998], Department of Chemistry, University of Rochester.
- ⋆ 1996 Graduate Student Award in Computational Chemistry supported by American Chemical Society Division of Physical Chemistry, the Subdivision of Theoretical Chemistry, IBM, and the Cornell Theory Center.
- ⋆ Elon Huntington Hooker Graduate Fellowship [1996-1997], Department of Chemistry, University of Rochester.
- ⋆ Sherman Clarke Fellowship [1996-1997], Department of Chemistry, University of Rochester.
- ⋆ 'Red Diploma' (Diploma with Honor), Moscow Institute of Physics and Technology, Dolgoprudny, Russia, June 1994.
- ⋆ Special Institute Fellowship [1992-1994], Moscow Institute of Physics and Technology, Dolgoprudny, Russia.

Professional Service

- ⋆ Organizer of the conference series in the Center for Nonlinear Studies at Los Alamos National Laboratory: *"Excited State Processes in Electronic and Bio Nanomaterials (ESP)"*, 2001, 2003, 2005, 2007.
- ⋆ Organizer of the Telluride workshop: *"Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy"*, Telluride, CO, 2007.
- ⋆ Co-organizer of the 27th CNLS Annual Conference *"Complexity of Biological and Soft Materials"*, Santa Fe, NM, 2007.
- ⋆ Organizer of the conference in the Center for Nonlinear Studies at Los Alamos National Laboratory: *"Electronic and Vibrational Interactions in Carbon Nanotubes"*, Santa Fe, NM, 2006
- ⋆ Co-organizer of the 24th CNLS Annual Conference *"Statistical Physics of Macromolecules: from electronic structure to fluid mechanics"*, Santa Fe, NM, 2004.
- ⋆ Member of LANL Postdoctoral Committee, Los Alamos National Laboratory, 2006-present.
- ⋆ Member of CNLS Executive Committee, Los Alamos National Laboratory, 2004-present.
- ⋆ Manager of the Theoretical Division P/T Colloquium series, Los Alamos National Laboratory, 2001-2005.

- ⋆ Member of LDRD-ER review committee in Quantum Science category, Los Alamos National Laboratory, 2007.
- ⋆ Member of LDRD-ER review committee in Chemistry and Materials category, Los Alamos National Laboratory, 2005.
- ⋆ Member of LDRD-ER review committee in Technology category, Los Alamos National Laboratory, 2004.
- ⋆ Member of CNLS public service committee, Los Alamos National Laboratory, 2001-2003.

Refereeing for Journals

Proceedings of the National Academy of Science
International Journal of Quantum Chemistry
Journal of the American Chemical Society
Journal of Chemical Theory and Computation
Journal of Physical Chemistry
Physical Chemistry Chemical Physics
Journal of Luminescence
Journal of Chemical Physics
Computational Materials Science
Applied Physics Letters
Physical Review A, B, C
Physics Review Letters
Chemical Physics Letters
Chemical Physics
Physics Letters A
Nanoletters
Science
Physica B, D
Macromolecules

Refereeing for Agencies

Petroleum Research Fund (PRF-ACS)
National Science Foundation (NSF)
US Department of State for the Science Centers
Office of Basic Energy Sciences (OBES) at DOE
John D. and Catherine T. MacArthur Foundation
Research Corporation Award Programs
Netherlands Foundation for Fundamental Research (FOM)
Laboratory-Directed Research and Development (LDRD)

Computer Experience

- System Administration and support services for a cluster of computer workstations (University of Rochester, Prof. Mukamel research group, 1996-1999)
- Programming languages: Fortran-77 (90), C(C++), Pascal, Basic, Perl.
- Computers: CRAY C90, SGI (Origin 2000, Octane, O2, Indigo, Power Indigo), DEC Alpha (264DP, EV56), Sun (Ultra, Ultra-2), IBM RS/6000 SP (Cornell Theory Center), Intel and AMD processors.
- Operating systems: IRIX, AIX, UNICOS, Digital Unix, Solaris, Linux, Dos, Windows (95/98/ME, NT/2000/XP).

- Computational Chemistry software: Gaussian, Gamess, Spartan, Turbomole, CS ChemOffice, Macromodel, Cambridge Structural Database, ZINDO, MOPAC, Hyperchem.
- Software Packages: Mathematica, Maple, Matlab, Microcal Origin, Microsoft Office, LaTex, Adobe Illustrator, Adobe Photoshop, Corel Draw.

Professional References

Professor Guillermo C. Bazan
Department of Chemistry
University of California
Santa Barbara CA 93106
E-mail: bazan@chem.ucsb.edu
(805) 893-5538 (Phone)
(805) 893 4120 (Fax)

Dr. Alan R. Bishop
Theoretical Division, MS B210
Los Alamos National Laboratory
Los Alamos, NM 87545
E-mail: arb@lanl.gov
(505) 667-4401 (Phone)
(505) 665-4055 (Fax)

Professor Jean-Luc Brédas
School of Chemistry and Biochemistry
Georgia Institute of Technology
Atlanta, GA 30332-0400
E-mail:
jean-luc.bredas@chemistry.gatech.edu
(404) 385-4986 (Phone)
(404) 894-7452 (Fax)

Professor Shaul Mukamel
Department of Chemistry
University of California, Irvine
433A Rowland Hall
Irvine, CA 92697-2025
E-mail: smukamel@uci.edu
(949) 824-7600 (Phone)
(949) 824-8571 (Fax)

Professor Anne B. Myers-Kelley
Division of Natural Sciences
University of California, Merced
P.O. Box 2039, Merced, CA 95344
E-mail: amkelley@ucmerced.edu
(209) 724-4309 (Phone)
(209) 724-4424 (Fax)

Dr. Sci. Victor Klimov
C-PCS, MS-J567
Los Alamos National Laboratory
Los Alamos, NM 87545
E-mail: klimov@lanl.gov
(505) 665-8284 (Phone)
(505) 667-0440 (Fax)

Professor Lewis Rothberg
Department of Chemistry
University of Rochester
Rochester NY 14627
rothberg@chem.rochester.edu
(716) 275-8286 (Phone)
(716) 473-6889 (Fax)

Professor Mark A. Ratner
Department of Chemistry
Northwestern University
Evanston, IL 60208
ratner@chem.northwestern.edu
(847) 491-5652 (Phone)
(847) 467-2447 (Fax)

Invited talks and presentations

- *"Theoretical spectroscopy and photoinduced dynamics of organic nano-materials"* (invited seminar), University of Michigan, Ann Arbor, MI, November 2007.
- *"Theoretical spectroscopy and photoinduced dynamics of organic nano-materials"* (invited seminar), Naval Research Laboratory, Washington DC, October 2007.
- *"A theoretical study of optical response and photodynamics in conjugated organic materials"* (invited talk), Conference on Molecular Photonics, Friday Harbor, WA, August 2007.
- *"Photoinduced dynamics and multiscale modeling on the nanoscale"* (invited talk), Telluride Workshop on Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, July 2007.
- *"Photoinduced dynamics in organic nano-materials and multiscale modeling of optical spectra using TDDFT"* (invited talk), 2007 Gordon Research Conference on Time-dependent Density Functional Theory, Waterville, ME, July 2007.
- *"Optical response and photodynamics of functional organic materials"* (invited seminar), Department of Chemistry, Norfolk State University, Norfolk, VI, May, 2007.
- *"Optical response and photodynamics of functional organic materials"* (invited seminar), Department of Chemistry and Biochemistry, Duke University, Durham, NC, May, 2007.
- *"Optical response and photodynamics of functional organic materials"* (invited seminar), Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY, April, 2007.
- *"Theoretical study of photoexcited dynamics in conjugated polymers and carbon nanotubes"* (invited talk), 233th ACS National Meeting, Chicago, IL, March 2007.
- *"Exciton scattering and localization in branched dendrimeric structures"* (talk), 233th ACS National Meeting, Chicago, IL, March 2007.
- *"Excitons and spectroscopy of carbon nanotubes and pi-conjugated polymers" and "Selected applications of quantum chemistry to functional optical materials"* (invited seminars), University of Mons Hainaut, Mons, Belgium, December, 2006.
- *"Selected applications of quantum chemistry to functional optical materials"* (invited seminar), Chemistry Department, Lund University, Lund, Sweden, December, 2006.
- *"Excitons and spectroscopy of carbon nanotubes and pi-conjugated polymers" and "Selected applications of quantum chemistry to functional optical materials"* (invited seminars), University de Rennes, Rennes, France, December, 2006.
- *"TD-DFT: selected applications to nanoscience"* (invited talk), COST conference, Paris, France, December, 2006.
- *"Selected applications of quantum chemistry to functional optical materials"* (invited seminar), Chemistry Department, Karlsruhe University, Karlsruhe, Germany, November, 2006.

- *"Photoinduced processes in conjugated polymers and carbon nanotubes: similarities and differences"* (invited seminar), Dipartimento di Fisica, Politecnico di Milano, Milano, Italy, November, 2006.
- *"Nonlinear optical response and photodynamics of substituted chromophores: a TDDFT study"* (invited talk), ICCMSE 2006, Ghania, Crete, Greece, October, 2006.
- *"Nonlinear optical response and photodynamics of conjugated molecules: effects of branching and substitution"* (invited GRA Theoretical Chemistry Lecture), MIT, Cambridge, MA, September 2006.
- *"Photoinduced processes in conjugated polymers and carbon nanotubes: similarities and differences"* (invited seminar), Department of Chemistry, Massachusetts Institute of Technology (MIT), Cambridge, MA, September 2006.
- *"Photoinduced processes in conjugated polymers and carbon nanotubes: similarities and differences"* (invited talk), 2006 Gordon Research Conference on Electronic Processes in Organic Materials, South Hadley, MA, July 2006.
- *"Single and Biexciton Binding Energy in Core/Shell Semiconductor Composite Nanocrystals: an Interplay of Quantum and Dielectric Confinement"* (invited talk), ICCE-14 (International Conference on Composites/Nano Engineering), Boulder, CO, July 2006.
- *"Conjugated polymers vs. carbon nanotubes or 1D: how big is enough?"* (brown bag seminar), T-12, Los Alamos National Laboratory, Los Alamos, NM, May 2006.
- *"Nonlinear optical response and photodynamics of conjugated molecules: effects of branching and substitution"* (invited seminar), Department of Physics, the University of Utah, Salt Lake City, UT, April 2006.
- *"Photoprocesses in conjugated polymers and carbon nanotubes: similarities and differences"* (invited seminar), Department of Chemistry, University of California at Irvine, Irvine, CA, April 2006.
- *"Excited state photodynamics in semiconducting polymers and their assemblies"* (invited talk), International Symposium on Semiconducting Polymers and Devices, Hsinchu, Taiwan, February 2006.
- *"Photoprocesses in conjugated polymers and carbon nanotubes: similarities and differences"* (invited seminar), Department of Chemistry, University of Washington, Seattle, WA, February 2006.
- *"Modeling of excited state dynamics and spectroscopy in large molecular clusters"* (invited talk), PacificChem 2005, Honolulu, Hawaii, December 2005.
- *"Electronic excitations and photodynamics in conjugated polymers and carbon nanotubes", "Adiabatic and nonadiabatic excited state dynamics in molecular aggregates", "Nonlinear optical response of organic electronic materials", "Electronic structure and interactions in colloidal quantum dots and their assemblies"* (invited lectures), Winter School in Theoretical Chemistry on Nanophotonics, Department of Chemistry, University of Helsinki, Helsinki, Finland, December 2005.

- *"Introduction to theoretical modeling of molecular excited states"* (invited seminar), Department of Chemistry, University of Rennes, Rennes, France, November 2005.
- *"Photophysics of conjugated polymers and carbon nanotubes: similarities and differences"* (invited seminar), Department of Chemistry, Wayne State University, Detroit, MI, September 2005.
- *"Adiabatic and nonadiabatic excited state dynamics in large molecular clusters"* (invited talk), 230th ACS National Meeting, Washington DC, August 2005.
- *"Effects of branching in substituted conjugated chromophores on photophysical properties and two-photon absorption"* (talk), 229th ACS National Meeting, San Diego, CA, March 2005.
- *"Nonlinear and nonadiabatic dynamics in coupled electron-phonon systems"* (invited talk), Telluride Workshop on Nonadiabatic Dynamics, Telluride, CO, August 2004.
- *"Excited states and nonlinear optical response of organic electronic materials"* (invited seminar), Department of Chemistry, the University of Southern California, Los Angeles, CA, May 2004.
- *"Excited states and nonlinear optical response of organic electronic materials"* (invited seminar), Department of Chemistry, the University of California, Davis, CA, April 2004.
- *"Electron-Vibrational Dynamics of Photoexcited Polyfluorenes"* (talk), *"Semiempirical methods for modeling of photoexcited dynamics in organic electronic materials"* (talk), 227th ACS National Meeting, Anaheim, CA, March 2004.
- *"Nonlinear optical response of organic electronic materials"* (invited lecture), Binational Consortium of Optics Winter School, Tucson, Arizona, January 2004.
- *"Electron-vibrational dynamics of photoexcited polyfluorenes"* (talk), XX Southwest Theoretical Chemistry Conference, Lubbock, Texas, November 2003.
- *"Nonlinear optical response of conjugated molecules: A TDDFT study"* (invited talk), The Third International Symposium on Optical Power Limiting, Sedona, Arizona, October 2003.
- *"Photoexcited breathers in pi-conjugated polymers. Do they exist?"* (invited talk), International CECAM conference on Modeling Electronic Processes in Molecular Scale Devices, Lion, France, September 2003.
- *"Photoexcited breathers in pi-conjugated polymers: an excited state molecular dynamics study"* (invited talk), 2003 Gordon Research Conference on Electronic Spectroscopy and Dynamics, Lewiston, ME, July 2003.
- *"Excited states, potentials, and nonlinear optical response of conjugated molecules"* (invited seminar), Department of Chemistry, the University of Texas at Austin, Austin, TX, April 2003.
- *"Excited states and nonlinear optical response of conjugated molecules: A TDDFT study"* (invited talk), 225th ACS National Meeting, New Orleans, LA, March 2003.

- *"Photoexcitation dynamics and defects in conjugated polymers: a quantum-chemical study"* (invited talk), 2002 MRS Fall National Meeting, Boston, MA, November 2002.
- *"Excited states, potentials, and nonlinear optical response of conjugated molecules"* (materials seminar), Theory Division, Los Alamos National Laboratory, Los Alamos, NM, October 2002.
- *"Excited states, potentials, and nonlinear optical response of conjugated molecules: TDDFT and RPA/semiempirical study"* (invited talk), conference on TDDFT methods at Wright-Patterson Air Force Base, Ohio, August 2002.
- *"Photoexcited conformational dynamics of conjugated polymers"* (invited talk), CNLS conference on Intrinsic Localized Modes, Los Alamos, NM, July 2002.
- *"Semiempirical/RPA approaches for excited state molecular electronic structure"* (invited talk), 2002 Gordon Research Conference on Computational Chemistry, New London, NH, June 2002.
- *"Excited state dynamics in Poly-phenylenevinylene (PPV) oligomers"* (talk), 2001 MRS Fall National Meeting, Boston, MA, November 2001.
- *"Semiempirical methods for excited state dynamics of conjugated molecules"* (talk), 221th ACS National Meeting, San Diego, CA, April 2001.
- *"Semiempirical methods for excited state molecular electronic structure"* (invited seminar), Department of Chemistry, Duke University, Durham, NC, February 2001.
- *"Excited-state dynamics of conjugated molecules"* (talk), Western Spectroscopy Association Conference, Pacific Grove, CA, February 2001.
- *"Semiempirical methods for excited state molecular electronic structure"* (invited seminar), Department of Chemistry, Chicago University, Chicago, IL, January 2001.
- *"Semiempirical methods for excited state molecular electronic structure"* (seminar), Department of Chemistry, Marquette University, Milwaukee, WI, January 2001.
- *"Semiempirical methods for excited state molecular electronic structure"* (invited seminar), Department of Chemistry, Clemson University, Clemson, SC, January 2001.
- *"Semiempirical methods for excited state molecular electronic structure"* (seminar), Department of Chemistry, Kansas State University, Manhattan, Kansas, November 2000.
- *"CEO/semiempirical calculations of excited electronic states in conjugated molecules"* (poster), *"Interchain electronic excitations in poly-phenylenevinylene (PPV) aggregates"* (poster), 2000 Gordon Research Conference on Electronic Processes in Organic Materials, Rhode Island, July 2000.
- *"Photosynthesis: Electronic excitations and energy transfer in the biological light-harvesting (LH) antenna complexes"* (seminar), Department of Chemistry, University of California at Santa Barbara, Santa Barbara, CA, May 2000.

- *"Photosynthesis: Electronic excitations and energy transfer in the biological light-harvesting (LH) antenna complexes"* (invited talk), Corning Incorporated, Corning, NY, April 2000.

- *"Excitonic couplings and electronic coherence in bridged naphthalene dimers"* (talk), APS National Meeting 2000, Minneapolis, MN, March 2000.

- *"CEO/semiempirical calculations of excited electronic states of conjugated molecules"* (talk), *"RPA/MOPAC calculations of excited state energies and adiabatic surfaces"* (talk), *"Frenkel exciton Hamiltonian for LH2 photosynthetic antenna"* (poster), 219th ACS National Meeting, San Francisco, CA, March 2000.

- *"Interchain Electronic Excitations in Poly-Phenylenevinylene (PPV) Oligomer and Polymer Aggregates"* (talk), *"Modeling Chromophore-Chromophore Interactions Using Paracyclophane Derivatives"* (talk), 4th International Topical Conference on Optical Probes of Conjugated Polymers and Photonic Crystals, Salt Lake City, Utah, February 2000.

- *"Exciton-Hamiltonian and Delocalized Electronic Excitations in the LH2 Antenna Complex of Purple Bacteria"* (talk), Department of Chemistry, University of Southern California, Los Angeles, CA, December 1999.

- *"Origin, Scaling, and Saturation of Nonlinear Polarizabilities in Donor/Acceptor Polymers"* (seminar), Los Alamos National Laboratory, Los Alamos, NM, November 1999.

- *"Localized and Delocalized Electronic Excitations in Biological and Artificial Antenna Complexes"* (invited talk), 10th annual Symposium, NSF Center for Photoinduced Charge Transfer, University of Rochester, Rochester, NY, July 1999.

- *"Electronic Spectroscopy of Conjugated and Aggregated Molecules"* (invited seminar), College of Chemistry, University of California at Berkeley, Berkeley, CA, January 1999.

- *"Collective Electronic Excitations in Spectroscopy of Conjugated and Aggregated Molecules"* (invited seminar), Los Alamos National Laboratory, Los Alamos, NM, January 1999.

- *"Frenkel Exciton Model for Optical Excitations in Fractal Antenna Supermolecules"* (seminar), the Rochester Theory Center for Optical Science and Engineering, University of Rochester, Rochester, NY, December 1998.

- *"Collective Electronic Excitations in Spectroscopy of Conjugated and Aggregated Molecules"* (seminar, PhD defense), Department of Chemistry, University of Rochester, Rochester, NY, November 1998.

- *"Localized Electronic Excitations in Phenylacetylene Dendrimers"* (poster), symposium on Electronic Properties in Organic Condensed Matter, NSF Center for Photoinduced Charge Transfer, University of Rochester, Rochester, NY, August 1998.

- *"Collective Electronic Excitations in Conjugated Molecules"* (poster), *"Collective Electronic Excitations in Aggregated Molecules"* (poster), 1998 Gordon Research Conference on Electronic Processes in Organic Materials, Rhode Island, July 1998.

- *“Collective Optical Excitations in Spectroscopy of Fractal Antenna Supermolecules”* (seminar), the Rochester Theory Center for Optical Science and Engineering NSF Site-Visit Panel, University of Rochester, Rochester, NY, June 1998.
- *“Collective Optical Excitations in Nonlinear Spectroscopy of Conjugated Molecules”* (talk), the Rochester Theory Center for Optical Science and Engineering Annual Symposium, University of Rochester, Rochester, NY, August 1997.
- *“Recursive Density-Matrix-Spectral-Moment Algorithm for Optical Properties of Conjugated Molecules”* (poster), 8th annual Symposium on Materials for Electronics and Imaging, NSF Center for Photoinduced Charge Transfer, University of Rochester, Rochester, NY, August 1996.
- *“Recursive Density-Matrix-Spectral-Moment Algorithm for Molecular Nonlinear Polarizabilities”* (poster), 1996 Gordon Research Conference on Electronic Processes in Organic Materials, Proctor Academy, New Hampshire, July 1996.
- *“Generalized Sum Rules and Dominant Electronic Oscillators for Nonlinear Response of Conjugated molecules”* (seminar), Department of Chemistry, University of Rochester, Rochester, NY, April 1996.

Publications

1. S. Tretiak, V. Chernyak, and S. Mukamel, ”Collective electronic oscillators for nonlinear optical response of conjugated molecules,” *Chem. Phys. Lett.*, **259**, 55-61 (1996).
2. S. Tretiak, V. Chernyak, and S. Mukamel, ”Chemical bonding and size scaling of nonlinear polarizabilities of conjugated polymers,” *Phys. Rev. Lett.*, **77**, 4656-4660 (1996).
3. S. Tretiak, V. Chernyak, and S. Mukamel, ”Recursive density-matrix-spectral-moment algorithm for molecular nonlinear polarizabilities,” *J. Chem. Phys.*, **105**, 8914-8928 (1996).
4. T. Meier, S. Tretiak, V. Chernyak, and S. Mukamel, ”Electronic-oscillator analysis of femtosecond four-wave mixing in conjugated polyenes,” *Phys. Rev. B*, **55**, 4960-4978 (1997).
5. S. Mukamel, S. Tretiak, Th. Wagersreiter, and V. Chernyak, ”Electronic coherence and collective optical excitations of conjugated molecules,” *Science*, **277**, 781-787 (1997).
6. S. Tretiak, V. Chernyak, and S. Mukamel, ”Two-dimensional real-space analysis of optical excitations in acceptor-substituted carotenoids,” *J. Am. Chem. Soc.*, **119**, 11408-11419 (1997).
7. S. Tretiak, V. Chernyak, and S. Mukamel, ”Origin, scaling, and saturation of second order polarizabilities in donor/acceptor polyenes,” *Chem. Phys. Lett.*, **287**, 75-82 (1998).
8. S. Tretiak, V. Chernyak, and S. Mukamel, ”Localized electronic excitations in phenylacetylene dendrimers,” *J. Phys. Chem. B*, **102**, 3310-3315 (1998).
9. G. C. Bazan, W. J. Oldham, Jr., R. J. Lachicotte, S. Tretiak, V. Chernyak, and S. Mukamel, ”Stilbenoid dimers: Dissection of a paracyclophane chromophore,” *J. Am. Chem. Soc.*, **120**, 9188-9204 (1998).

10. S. Tretiak, V. Chernyak, and S. Mukamel, "Excited electronic states of carotenoids: Time-dependent density-matrix-response algorithm," *Int. J. Quant. Chem.*, **70**, 711-727 (1998).
11. S. Tretiak, V. Chernyak, and S. Mukamel, "Real-space analysis of electronic excitations in free-base (H_2P) and magnesium (MgP) porphins," *Chem. Phys. Lett.*, **297**, 357-364 (1998).
12. S. Tretiak, "Collective Electronic Excitations in Spectroscopy of Conjugated and Aggregated Molecules," *Ph.D. Thesis*, University of Rochester (1999).
13. E. V. Tsiper, V. Chernyak, S. Tretiak, and S. Mukamel, "Ground-State-Density-Matrix Algorithm for Excited State Adiabatic Surfaces; Application to Polyenes," *Chem. Phys. Lett.*, **302**, 77-84 (1999).
14. E. Poliakov, V. Chernyak, S. Tretiak, and S. Mukamel, "Exciton-scaling and optical excitations of self-similar phenylacetylene dendrimers," *J. Chem. Phys.*, **110**, 8161-8175 (1999).
15. E. V. Tsiper, V. Chernyak, S. Tretiak, and S. Mukamel, "Density-matrix-spectroscopic algorithm for excited-state adiabatic surfaces and molecular dynamics of a protonated Schiff base," *J. Chem. Phys.*, **110**, 8328-8337 (1999).
16. S. Tretiak, V. Chernyak, and S. Mukamel, "Electronic screening in second order optical polarizabilities of elongated Donor/Acceptor polyenes," *Chem. Phys.*, **245**, 145-163 (1999).
17. J. Ern, A. T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. Tsiper and C. Kryschi, "Reaction dynamics of photochromic dithienylethene derivates," *Chem. Phys.*, **246**, 115-125 (1999).
18. V. Chernyak, E. Poliakov, S. Tretiak, and S. Mukamel, "Localized optical excitations and two-exciton spectroscopy of phenylacetylene Dendrimers," in Dynamics in Small Confining Systems IV, *Mat. Res. Soc. Proc.*, J. M. Drake, G. S. Grest, J. Klafter, and R. Kopelman Eds., vol. **543**, 327 (1999).
19. V. Chernyak, E. Poliakov, S. Tretiak, and S. Mukamel, "Two-exciton states and spectroscopy of phenylacetylene dendrimers," *J. Chem. Phys.*, **111**, 4158-4168 (1999).
20. S. Tretiak, W. M. Zhang, V. Chernyak, and S. Mukamel, "Excitonic couplings and electronic coherence in bridged naphthalene dimers," *Proc. Nat. Acad. Sci. USA*, **96**, 13003-13008 (1999).
21. M. Schulz, S. Tretiak, V. Chernyak, and S. Mukamel, "Size scaling of third-order off-resonant polarizabilities; Electronic coherence in organic oligomers," *J. Am. Chem. Soc.*, **112**, 452-459 (2000).
22. S. Wang, G. C. Bazan, S. Tretiak, and S. Mukamel, "Oligophenylenevinylene Phane dimers: Probing the effect of contact site on the optical properties of bichromophoric pairs," *J. Am. Chem. Soc.*, **122**, 1289-1297 (2000).
23. A. Piryatinski, S. Tretiak, V. Chernyak, and S. Mukamel, "Simulations of two- dimensional femtosecond infrared photon-echoes of glycine gipeptide," *J. Raman Spect.*, **31**, 125-135 (2000).
24. V. Chernyak, S. Tretiak, and S. Mukamel, "Electronic versus vibrational optical nonlinearities of push-pull polymers," *Chem. Phys. Lett.*, **319**, 261-264 (2000).

25. J. Ern, A. T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. V. Tsiper, and C. Kryschi, "Femtosecond reaction dynamics of a photochromic dithienylethene derivative," *J. Lum.*, **87-9**, 742-744 (2000).
26. T. Minami, S. Tretiak, V. Chernyak, and S. Mukamel, "Frenkel-exciton Hamiltonian for dendrimeric nanostar," *J. Lum.*, **87-9**, 115-118 (2000).
27. S. Tretiak, C. Middleton, V. Chernyak, and S. Mukamel, "Exciton Hamiltonian for the Bacteriochlorophyll System in the LH2 Antenna Complex of Purple Bacteria," *J. Phys. Chem. B*, **104**, 4519-4528 (2000).
28. S. Tretiak, "Effective Computing at CNLS," (2000), Published on Web: http://cnls.lanl.gov/Internal/Computing/Software/cnls_computation_ug.pdf.
29. V. Chernyak, S. Tretiak, M. Schulz, E. V. Tsiper, and S. Mukamel, "Krylov-space algorithms for time-dependent HartreeFock and density functional computations," *J. Chem. Phys.*, **113**, 36-43 (2000).
30. S. Tretiak, C. Middleton, V. Chernyak, and S. Mukamel, "Localized and Delocalized Electronic Excitations in Biological and Artificial Antenna Complexes," in *Photoinduced Charge Transfer*, L. Rothberg, Editor (World Scientific, 2000).
31. V. Chernyak, S. Tretiak, E. V. Tsiper, T. Meier, and S. Mukamel, "Semiclassical Effective Hamiltonian for Coupled Electronic and Nuclear Optical Response," *CMT22 Workshop Proc., Vol. 14, Condensed Matter Theories*, Vanderbilt University, D. Ernst, Editor (2001).
32. S. Tretiak, A. Saxena, R. L Martin, and A. R. Bishop, "Interchain Electronic Excitations in Poly-Phenylenevinylene (PPV) Aggregates," *J. Phys. Chem. B*, **104**, 7029-7037 (2000).
33. S. Tretiak, C. Middleton, V. Chernyak, and S. Mukamel, "Bacteriochlorophyll and Carotenoid Excitonic Couplings in the LH2 System of Purple Bacteria," *J. Phys. Chem. B*, **104**, 9540-9553 (2000).
34. S. Tretiak, A. Saxena, R. L Martin, and A. R. Bishop, "CEO/semiempirical calculations of uv-visible spectra in conjugated molecules," *Chem. Phys. Lett.*, **331**, 561-568 (2000).
35. J. Ern, A.T. Bens, H.-D. Martin, S. Mukamel, S. Tretiak, K. Tsyganenko, K. Kuldova, H.P. Trommsdorff, C. Kryschi, "Reaction dynamics of a photochromic fluorescing dithienylethene," *J. Phys. Chem. A*, **105**, 1741-1749 (2001).
36. S. Tretiak, R. L. Martin, A. Saxena, and A. R. Bishop, "CEO/semiempirical calculations of static nonlinear polarizabilities in conjugated molecules," *J. Chem. Phys.*, **115**, 699-707 (2001).
37. S. Tretiak, "Random phase approximation/semiempirical computations of electronic structure of extended organic molecules" Chapter in *Recent Research Developments in Physical Chemistry*, 5th issue, India, (2001).
38. I. H. Campbell, D. L. Smith, S. Tretiak, R. L. Martin, C. J. Neef and J. P. Ferraris, "Excitation transfer processes in a phosphor-doped poly(p-phenylene vinylene) light-emitting diode," *Phys. Rev. B*, **6508**, 5210-5210 (2002).
39. S. Tretiak, R. L. Martin, A. Saxena, and A. R. Bishop, "Conformational dynamics of photoexcited conjugated molecules," *Phys. Rev. Lett.*, **89**, 97402-97406 (2002).

40. S. Tretiak and S. Mukamel, "Density matrix analysis and simulation of electronic excitations in conjugated and aggregated molecules," *Chem. Rev.*, **102**, 3171-3212 (2002).

41. S. A. Crooker, J. Hollingsworth, S. Tretiak, and V. I. Klimov, "Spectrally resolved dynamics of energy transfer in quantum-dot assemblies: Towards engineered energy flows in artificial materials," *Phys. Rev. Lett.*, **89**, 6802-6802 (2002).

42. K. A. Nguyen, R. Pachter, S. Tretiak, V. Chernyak, and S. Mukamel, "Analysis of absorption spectra of zinc porphyrin, zinc meso-tetraphenylporphyrin, and halogenated derivatives," *J. Phys. Chem.*, **106**, 10285-10293 (2002).

43. S. Tretiak, R. L. Martin, A. Saxena, and A. R. Bishop, "Geometry relaxation of photoexcited states in conjugated molecules," *Phase Transitions*, **75**, 725-732 (2002).

44. A. M. Moran, A. Myers Kelley, and S. Tretiak, "Excited state molecular dynamics simulations of nonlinear pushpull chromophores," *Chem. Phys. Lett.*, **367**, 293-307 (2003).

45. S. Tretiak, R. L. Martin, A. Saxena, and A. R. Bishop, "Photoexcited breathers in conjugated polyenes: An excited state molecular dynamics study," *Proc. Nat. Acad. Sci. USA*, **100**, 2185-2190 (2003).

46. I. Franco and S. Tretiak, "Photoexcitation dynamics of polyfluorenes in the presence of chemical defects: a theoretical study," *Chem. Phys. Lett.*, **372**, 403-408 (2003).

47. S. Tretiak and V. Chernyak, "Resonant nonlinear polarizabilities in the time-dependent density functional (TDDFT) theory," *J. Chem. Phys.*, **119**, 8809-8823 (2003).

48. S. Tretiak, R. L. Martin, A. Saxena, and A. R. Bishop, "Photoexcitation dynamics in polyconjugated molecules," *Attidella Fondazione Giorgio Ronchi*, ANNO-LVIII, **6**, 819-828 (2003).

49. A. Masunov and S. Tretiak, "Prediction of two photon absorption properties for the large organic molecules using the time-dependent density functional theory," *J. Phys. Chem. B*, **108**, 899-907 (2004).

50. N. Kobko, A. Masunov and S. Tretiak, "Calculations of the third-order nonlinear optical responses in push-pull chromophores with a time-dependent density functional theory," *Chem. Phys. Lett.*, **392**, 444-451 (2004).

51. S. A. Ivanov, J. Nanda, A. Piryatinski, M. Achermann, L. P. Balet, I. V. Bezel, P. O. Anikeeva, S. Tretiak, and V. I. Klimov, "Light amplification using inverted core/shell nanocrystals: towards lasing in the single-exciton regime", *J. Phys. Chem. B*, **108**, 10625-10630 (2004).

52. G. P. Bartholomew, M. Rumi, S. J. K. Pond, J. W. Perry, S. Tretiak and G. C. Bazan "Two-photon absorption in three-dimensional chromophores Based on [2.2] - Paracyclophane," *J. Am. Chem. Soc.*, **126**, 11529-11542 (2004).

53. I. Franco and S. Tretiak, "Electron-vibrational dynamics of photoexcited polyfluorenes," *J. Am. Chem. Soc.*, **126**, 12130-12140 (2004).

54. A. Piryatinski, S. Tretiak, A. Saxena, R. L. Martin, and A. R. Bishop "Three-pulse photon-echo spectroscopy as a probe of the photoexcited electronic state manifold in coupled electron-phonon system", *Phys. Rev. B (Rapid Comm.)*, **70**, 161404-161407 (2004).

55. S. Tretiak, A. Piryatinski, A. Saxena, R. L. Martin, and A. R. Bishop, "On the existence of photoexcited breathers in conducting polymers," *Phys. Rev. B*, **70**, 233203-233206 (2004).
56. R. J. Magyar, S. Tretiak, Y. Gao, H.-L. Wang and A. P. Shreve, "A joint theoretical and experimental study of phenylene-acetylene molecular wires", *Chem. Phys. Lett.*, **401**, 149-156 (2005).
57. S. Tretiak, K. Igumenshchev and V. Chernyak, "Exciton sizes of conducting polymers predicted by time-dependent density functional theory", *Phys. Rev. B*, **71**, 033201-033204 (2005).
58. C. Katan, L. Porrs, O. Mongin, M. H. V. Werts, F. Terenziani, T. Pons, J. Mertz, S. Tretiak, and M. Blanchard-Desce, "Effects of (multi)branching of dipolar chromophores on photophysical properties and two-photon absorption," *J. Phys. Chem. A*, **109**, 3024-3037 (2005).
59. A. Masunov, S. Tretiak, J. W. Hong, B. Liu, and G. C. Bazan, "Theoretical study of the effects of solvent environment on photophysical properties and electronic structure of paracyclophane chromophores", *J. Chem. Phys.*, **122**, 224505 (2005).
60. E. A. Badaeva, T. V. Timofeeva, A. Masunov, S. Tretiak, "Role of donor-acceptor strengths and separation on the two-photon absorption response of cytotoxic dyes: a TD-DFT study," *J. Phys. Chem. A*, **109**, 7276-7284 (2005).
61. C. Katan, F. Terenziani, C. Le Droumagueta, O. Mongina, M. H. V. Wertsa, S. Tretiak, and Mireille Blanchard-Desce, "Branching of dipolar chromophores: effects on linear and nonlinear optical properties," Proc. SPIE Vol. 5935, p. 1-15 in Linear and Nonlinear Optics of Organic Materials V; Ed. Manfred Eich (2005).
62. A. Piryatinski, M. Stepanov, S. Tretiak, and V. Chernyak, "Semiclassical scattering on conical intersections", *Phys. Rev. Lett.*, **70**, 223001-223005 (2005).
63. J. F. Kauffman, J. M. Turner, I. V. Alabugin, B. Breiner, E. A. Badaeva, A. Masunov, and S. Tretiak, "Two-photon excitation of substituted enediynes", *J. Phys. Chem. A*, **110**, 241-251 (2006).
64. J. Nanda, S. A. Ivanov, H. Htoon, I. Bezel, A. Piryatinski, S. Tretiak, and V. I. Klimov, "Absorption cross sections and Auger recombination lifetimes in inverted core-shell nanocrystals: Implications for lasing performance", *J. Appl. Phys.*, **99**, 034309 (2006).
65. A. Gambetta, C. Manzoni, E. Menna, M. Meneghetti, G. Cerullo, G. Lanzani, S. Tretiak, A.Piryatinski, A. Saxena, R.L. Martin and A.R. Bishop, "Real time observation of non-linear vibrational dynamics in semiconducting single wall carbon nanotubes," *Nature Phys.*, **2**, 515-520 (2006).
66. C. Wu, S. Malinin, S. Tretiak, and V. Chernyak, "Exciton scattering and localization in branched dendrimeric structures," *Nature Phys.*, **2**, 631 - 635 (2006).
67. Z. Tang, R. K. Hicks, R. J. Magyar, S. Tretiak, Y. Gao, H.-L. Wang, "Synthesis and Characterization of Amphiphilic Phenylene-Ethynylene Oligomers and Their Langmuir-Blodgett Films", *Langmuir*, **22**, 8813-8820 (2006).
68. A. Piryatinski and S. Tretiak, "Effect of Quantum and Dielectric Confinements on the Exciton-Exciton Interaction Energy in Type-II Core/Shell Semiconductor Nanocrystals", SPIE Newsroom **8**, 384 (2006).

69. S. Tretiak, S. Kilina, A.Piryatinski, A. Saxena, R.L. Martin and A.R. Bishop, "Excitons and Peierls distortion in conjugated carbon nanotubes", *Nano Letters*, **7**, 86 - 92 (2007).

70. A. Piryatinski, S.A. Ivanov, S. Tretiak, and V.I. Klimov, "Effect of Quantum and Dielectric Confinement on the Exciton-Exciton Interaction Energy in Type-II Core/Shell Semiconductor Nanocrystals", *Nano Letters*, **7**, 108 - 115 (2007).

71. C. Wu, S. Tretiak, and V. Chernyak, "Excited states and optical response of a donor-acceptor substituted polyene: a TD-DFT study", *Chem. Phys. Lett.*, **433**, 305 - 311 (2007).

72. A.P. Shreve, E.H. Haroz, S.M. Bachilo, R.B. Weisman, S. Tretiak, S. Kilina, and S.K. Doorn, "Determination of Exciton-Phonon Coupling Elements in Single-Walled Carbon Nanotubes by Raman Overtone Analysis", *Phys. Rev. Lett.*, **98**, 037405 (2007).

73. P.T. Araujo, S.K. Doorn, S. Kilina, S. Tretiak, S. Maruyama, H. Chacham, M.A. Pimenta and A. Jorio, "Study of the third and fourth optical levels in carbon nanotubes", *Phys. Rev. Lett.*, **98**, 067401 (2007).

74. A. Tamulis, V. I. Tsifrinovich, S. Tretiak, G. P. Berman, D. L. Allara, "Neutral Radical Molecules Ordered in Self-Assembled Monolayer Systems for Quantum Information Processing", *Chem. Phys. Lett.*, **436**, 144 - 149 (2007).

75. R. J. Magyar and S. Tretiak, "The implications of spurious charge-transfer in TDDFT on the accurate description of large molecules and clusters", *J. Chem. Theory and Comput.*, **3**, 976 - 987 (2007).

76. A. Piryatinski, S. Tretiak, T.D. Sewell, and S.D. McGrane, "Vibrational spectroscopy of polyatomic materials: Semiempirical calculations of anharmonic couplings and IR Raman linewidth in naphthalene and PETN crystals", *Phys. Rev. B*, **75**, 214306 - 214315 (2007).

77. C. Katan, F. Terenziani, C. Droumaguet, O. Mongin, M.H.V. Werts, A. Bain, E. Badaeva, S. Tretiak, and M. Blanchard-Desce, "Two-photon transitions in quadrupolar and branched chromophores: experiment and theory", *J. Phys. Chem. A*, **111**, 9468 - 9483 (2007).

78. S. Tretiak, "Triplet absorption in carbon nanotubes: a TD-DFT study", *Nano Letters* (journal cover page), **7**, 2201-2206 (2007).

79. G.D. Scholes, S. Tretiak, T.J. McDonald, W.K. Metzger, C. Engtrakul, G. Rumbles, and M.J. Heben, "Low-lying exciton states determine the photophysics of semiconducting single wall carbon nanotube", *J. Phys. Chem. C* (journal cover page), **111**, 11139 - 11149 (2007).

80. S.A. Ivanov, A. Piryatinski, J. Nanda, S. Tretiak, K. R. Zavadil, W. O. Wallace, D. Werder, V.I. Klimov, "Type-II Core/Shell CdS/ZnSe nanocrystals: Synthesis, electronic structures, and spectroscopic properties", *J. Am. Chem. Soc.*, **129**, 11708 - 11719 (2007).

81. Z. Tang, N. Caculitan, M.S. Johal, P. Scudder, R.J. Magyar, S. Tretiak, and H.-L. Wang, "A Study of the Non-Covalent Interactions in Langmuir-Blodgett Films: An Interplay Between and Dipole-Dipole Interactions", *Thin Solid Films*, **516**, 58 - 66 (2007).

82. K. Igumenshchev, S. Tretiak, and V. Chernyak, "Excitonic effects in a time-dependent density functional theory", *J. Chem. Phys.*, **127**, 114902 (2007).

83. S. Kilina, S. Tretiak, D. Yarotskii, J.X. Zhu, N. Modine, A. Taylor and A.V. Balatsky, "Electronic properties of DNA base molecules adsorbed on a metallic surface", *J. Phys. Chem. C*, **111**, 14541 - 14551 (2007).

84. S. Kilina and S. Tretiak, "Excitonic and vibrational properties of single-walled semiconducting carbon nanotubes", *Adv. Func. Mat.* (Feature Article, journal cover page), **17**, 3405-3420 (2007).

85. P. Yang, E. Batista, A. Saxena, R.L. Martin, S. Tretiak and D.L. Smith "Effect of intra-molecular disorder and inter-molecular electronic Interactions on the electronic structure of poly-p-phenylene vinylene (PPV)", *Phys. Rev. B* (Rapid Comm.), **76**, 241201 (2007).

86. E. Badaeva and S. Tretiak, "Two photon absorption of extended substituted phenylenevinylene oligomers: a TDDFT study", *Chem. Phys. Lett.* **450**, 322328 (2008).

87. A. Piryatinski, S. Tretiak, and V. Chernyak, "Dynamical variational approach to non-adiabatic electronic structure", *Chem. Phys.* (in press).

88. C. Wu, S. Malinin, S. Tretiak, and V. Chernyak, "Multiscale Modeling of Electronic Excitations in Branched Conjugated Molecules Using Exciton Scattering Approach," *Phys. Rev. Lett.* (in press).

89. J. Tao, S. Tretiak, and J.-X. Zhu, "Performance of a non-empirical meta-GGA density functional for excitation energies", *J. Chem. Phys.* (in press).

90. Z. Rinkevicius, G. P. Berman, D. L. Allara, V. I. Tsifrinovich, and S. Tretiak "Characteristic parameters and dynamics of two-qubit system in self-assembled monolayers," (submitted).

91. K. Becker, E. Da Como, J. Feldmann, F. Scheliga, E. Thorn Csnyi, S. Tretiak, J.M. Lupton, "How chromophore shape controls photophysical function in phenylene-vinylenes", (submitted).

92. M. Galperin and S. Tretiak, "Linear optical response of current-carrying molecular junction: A NEGF-TDDFT approach", (submitted).

93. S. Kilina, S. Tretiak, S.K. Doorn, Z. Luo, F. Papadimitrakopoulos, A. Piryatinski, A. Saxena, R.L. Martin, and A.R. Bishop, "Cross-polarized Excitons of Carbon Nanotubes", (submitted).

94. S. Tretiak and R. L. Martin, "Excited state structure of photoluminescent polymers: a TDDFT study," (in preparation).

95. S. Tretiak and V. Chernyak, "Time-Dependent Density Functional Theory (TDDFT) in Finite-Dimensional Single-Orbital Spaces," (in preparation).

96. A. Piryatinski, S. Tretiak, H. Htoon, and V. I. Klimov, "Multiparticle Electronic Dynamics in Transition from Zero to One Dimension in Semiconductor Nanostructures", (in preparation).