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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/

Date of birth:	11/02/68
Place of birth:	Mariupol, Ukraine
Citizenship:	Russia
Status in the USA:	Permanent Resident

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; Molecular dynamics of the excited states; Collective electronic excitations and optical response of confined excitons in conjugated polymers, 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

March 2001 – Present	Technical Staff Member, Theoretical Chemistry and Molecular Physics T-12 Group of Theoretical Division, Los Alamos National Laboratory.
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.
December 1998 – July 1999	Postdoctoral Associate Group of Prof. Shaul Mukamel, Department of Chemistry, University of Rochester.
September 1994 – November 1998	Graduate Student Group of Prof. Shaul Mukamel, Department of Chemistry, University of Rochester.
September 1994 – May 1996	Graduate Teaching Assistant Department of Chemistry, University of Rochester.
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.

Public 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.
- ⋆ Co-organizer of the 24th CNLS Annual Conference *"Statistical Physics of Macromolecules: from electronic structure to fluid mechanics"*, Santa Fe, NM, 2004.
- ⋆ Management of the Theoretical Division P/T Colloquium series, Los Alamos National Laboratory, 2001-2004.
- ⋆ Member of CNLS public service committee, Los Alamos National Laboratory, 2001-present.

Referring for Journals

Proceedings of the National Academy of Science	Physics Review Letters
International Journal of Quantum Chemistry	Chemical Physics Letters
Journal of the American Chemical Society	Chemical Physics
Journal of Physical Chemistry	Physics Letters A
Journal of Chemical Physics	Science
Computational Materials Science	Physica B, D
Physical Review	Macromolecules

Computer Experience

- ◦ System Administration and support services for a cluster of computer workstations interconnected via TCP/IP: SGI Octane under IRIX 6.4, 3 SGI Indigo under IRIX 4.0.5, 7 dual boot Pentium III (II) PC clones under Linux (Slackware) $\Longleftrightarrow$ Windows-95 (98) (or NT 4.0), and two printers. (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 *86 compatible PCs.
- Operating systems: IRIX, AIX, UNICOS, Digital Unix, Solaris, Linux, Dos, Windows (95/98/ME, NT/2000/XP).
- Computational Chemistry software: Gaussian, Gamess, Spartan, CS ChemOffice, Macromodel, Rasmol, Cambridge Structural Database, ZINDO, MOPAC, Hyperchem.
- Software Packages: Mathematica, Maple, Matlab, Microcal Origin, Microsoft Office, LaTex, Adobe Illustrator, Adobe Photoshop, Corel Draw.

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 Gerald J. Small
Department of Chemistry
Iowa State University
Ames, IA 50011
gsmall@ameslab.gov
(515) 294-3859 (Phone)
(515) 294-1699 (Fax)

Invited talks and presentations

- *"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"* (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), 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"* (talk), 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. 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.*, **108**, 899-907 (2004).
49. 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).
50. J. Y. Lee, S. Tretiak, S. Volkov, G. C. Bazan, J. Zyss, and Shaul Mukamel, "Through-space charge transfer effects in two-photon absorption," *J. Chem. Phys.* (in press).
51. G. P. Bartholomew, M. Rumi, S. J. 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.*, (in press).
52. 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," (submitted).
53. A. Piryatinski, S. Tretiak, A. Saxena, R.L. Martin, and A.R. Bishop "Non-adiabatic dynamics in electron phonon coupled system", (submitted).
54. I. Franco and S. Tretiak, "Electron-Vibrational Dynamics of Photoexcited Polyfluorenes," (submitted).
55. S. Tretiak, K. Igumenshchev and V. Chernyak, "Exciton Sizes in Conducting Polymers described by Time-Dependent Density Functional Theory", (submitted).
56. N. Kobko, A. Masunov and S. Tretiak, "Study of nonlinear optical response in substituted stilbenes with the time-dependent density functional theory," (in preparation).
57. S. Tretiak, R. L. Martin, A. Saxena, and A. R. Bishop, "Modeling of Excited State Dynamics in Large Conjugated Molecules," (in preparation).
58. S. Tretiak and R. L. Martin, "Excited state structure of photoluminescent polymers: a TDDFT study," (in preparation).
59. S. Tretiak, "Exciton-Hamiltonian for the Bacteriochlorophyll System in the LH2 Complex of Purple Bacteria: TDDFT study," (in preparation).
60. T. Humble and S. Tretiak, "Quantum dots: surface reconstruction and passivation of ground state structures," (in preparation).
61. S. Tretiak, R. L. Martin, A. Saxena, and A. R. Bishop, "CEO/semiempirical calculations of excited states adiabatic potential surfaces," (in preparation).
62. S. Tretiak, R. L. Martin, A. Saxena, and A. R. Bishop, "Chaos in photoexcited dynamics of conducting polyenes," (in preparation).
63. S. Tretiak and V. Chernyak, "Time-Dependent Density Functional Theory (TDDFT) in Finite-Dimensional Single-Orbital Spaces," (in preparation).
64. 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).
65. B. Liu, B. Kohler, A. Mikhailovsky, G. C. Bazan, A. Masunov and S. Tretiak, "Solvent Effects on Water-Soluble Two Photon Absorption Chromophores", (in preparation).

66. J. W. Hong, G. C. Bazan, A. Masunov and S. Tretiak, "Photophysics and Electronic Structure of a Water-Soluble Paracyclophane", (in preparation).