

Sergei Tretiak

Theoretical Division, T-1/CINT, Mail Stop B221, Los Alamos National Laboratory, Los Alamos, NM
Phone: (505) 667-8351, E-mail: serg@lanl.gov; Web: <http://cnls.lanl.gov/~serg>

Professional employment history:

2017 – Present Deputy Group Leader at T-1, Theoretical Division, LANL
2001 – Present Technical Staff Member, Theoretical Division, LANL (Scientist Level 5)
2005 – Present Staff Scientist, Center for Integrated Nanotechnologies (CINT), LANL/SNL
2015 – Present Adjunct Professor at the University of California, Santa Barbara, CA
2015 – Present Adjunct Professor at Skolkovo Institute of Science & Technology (Russia)
2013 – 2015 Founding Faculty Fellow at Skolkovo Institute of Sci & Technology (Russia)
2006 – 2007 CNRS invited professor position, UMR 6510, University of Rennes, France
1999 – 2001 Director's Postdoctoral Fellow, Theoretical Division, LANL
1994 – 1998 Graduate Student, University of Rochester (Rochester, NY)
1991 – 1994 Graduate Student, Institute of Spectroscopy of Russian Academy of Sciences

Academic background:

1999 Ph.D. in Chemistry, University of Rochester (Rochester, NY); Advisor: Prof. Shaul Mukamel
1994 M.S. in Physics (Highest Honors), Institute of Physics and Technology (Moscow, Russia)

Professional Awards and Honors:

Fellow of the Royal Society of Chemistry, FRSC (2019); LANL Fellow (2018), Visiting Lecturer CRC Center at the University of Heidelberg, Germany (2018), LANL Postdoctoral Distinguished Mentor (2015), APS Fellow (2014), LANL Fellows Prize (2010), Slansky Fellow Award (2001), LANL Director's Postdoctoral Fellow (1999-2001), Arnold Weissberger Fellow (1997-1998), Graduate Student Award in Computational Chemistry, ACS (1996), Elon Huntington Fellow (1996-1997), Sherman Clarke Fellow (1996-1997), Diploma with Honor, Moscow Institute of Physics and Technology (1994).

Research interests:

Relation between optical and chemical properties of organic and semiconductor electronic functional materials; Charge and energy transfer in biological and artificial antenna complexes; Energy security and photovoltaic technologies, 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 electronically excited states; Collective electronic excitations and optical response of confined excitons in conjugated polymers, carbon nanotubes, semiconductor nanoparticles, mixed halide perovskites and molecular aggregates; Ultrafast nonlinear spectroscopy; Nonlinear dynamics of complex classical and quantum systems; Machine Learning and Data Science to complement conventional quantum chemistry toward modeling optical and chemical properties.

Highlights of professional service

- Organizer of the session "*Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters*" for the International Pacificchem conference, Honolulu, Hawaii, December 2015, December 2021.
- Founding organizer of the conference series at the Center for Nonlinear Studies (CNLS), LANL: "*Excited State Processes in Electronic and Bio Nanomaterials (ESP)*", 2001, 2003, 2005, 2007, 2009, 2011, 2014, 2016, 2018 and 2022.
- Co-organizer of the Telluride workshop series: "*Machine Learning and Informatics for Chemistry and Materials*", Telluride, CO, 2017, 2019, 2021.
- Organizer of Telluride workshop series on "*Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy*", Telluride, CO, 2007, 2009, 2011, 2013, 2015, 2017, 2021.
- Co-organizer Multidisciplinary Program Planning Group on "*Computational Materials and Nanoscience: Theory meets experiment*" and Co-organizer of the focused symposium "*Frontiers in Solar Light Harvesting Processes*" for the 251st ACS National Meeting, San Diego, CA, March 2016.
- Co-organizer the 2016 Mesilla Chemistry Workshop on "*Electrochemical Processes: Photovoltaics and Charge Transfer in Nanomaterials*" Mesilla, New Mexico, USA, January 2016.
- Co-organizer of the session "Physical Chemistry of Interfaces and Nanomaterials" for the SPIE Nano Science and Engineering conference, San Diego, CA, 2007-2018.
- Organizer of the CNLS Conferences: "*Physics Informed Machine Learning*", Santa Fe, NM, 2016, 2018 "*Statistical Physics of Macromolecules: from electronic structure to fluid mechanics*", Santa Fe, NM,

2004; "Electronic and Vibrational Interactions in Carbon Nanotubes", Santa Fe, NM, 2007; "Energy for 21st century", Santa Fe, NM, 2009.

- Member of LANL Postdoctoral Committee, Los Alamos National Laboratory, 2006-2009.

- Member of LANL LDRD-ER review committee in Quantum & Optical Science (2011-2013), Chemistry and Materials category (2005), in Technology category (2004).

- Member of CNLS Executive Committee, Los Alamos National Laboratory, 2004-present.

- Reviewer for over 30 major peer-reviewed journals and several funding agencies (NSF, Petroleum Research Fund (ACS), DOE BES, US Department of State for the Science Centers, *etc.*).

- Member of Proposal Evaluation Board at DOE Nanocenters, CFN (2012-14) and CNM (2016-2019).

- Affiliations ACS/APS/MRS/OSA/ECS/AAAS.

Mentoring: 31 postdocs (A. Masunov, 2001-04, now faculty at USF; R. Magyar, 2003-05, now TSM at SNL; A. Piryatinski, 2002-06, now TSM at LANL; S. Goupalov, 2003-04, now faculty at JSU; M. Lucero, 2005-06; M. Galperin, 2007-08, now faculty at UCD; J. Tao, 2007-10, now faculty at Tulane U; S. Kilina, 2008-10, now faculty at NDSU; K. Velizhanin, 2010-12, now TSM at LANL; H. Li, 2011-14, now postdoc at U Houston; A. Zhugayevych, 2011-14, now faculty at Skoltech, Moscow; A. Roslyak, 2012-14, now faculty at Fordham U; T. Nelson, Feynman Fellow, 2013-16, now TSM at LANL; L. Adamska, 2013-16, now postdoc at Padova; A. White, 2014-17, now TSM at LANL; J. Bjorgaard, 2013-16, now Scientist at TerraPower LLC; A. Neukirch, 2014-17, now TSM at LANL; B. Nebgen, 2016-18, now TSM at LANL; L. Zhou, 2017-2019, now faculty at UESTC, Chengdu, China; Y. Zhang, 2018-2019, now TSM at LANL; B. Gifford, 2018-2019, now TSM at LANL; J. Smith, Metropolis Fellow 2018-2020, now TSM at LANL; D. Ghosh, 2018-2021, now faculty at IIT Delhi, India; H. Tsai; Oppenheimer Fellow, 2019-2020, now scientist at First Solar; Galen Graven, Director Fellow, 2019-2021, now TSM at LANL; Dan Liu, 2020-2020, now faculty at Southeast University, China; Walter Malone, 2019-2021, now faculty at Tuskegee University; H. Song, 2019-present; Guoqing Zhou, 2020-present; Ashutosh Kumar, 2021-present; Adela Habib, 2021-present). Mentored over 100 students at LANL.

Selected invited and keynote talks (out of over 300):

ACS National Fall Meeting, Atlanta, GA (2021); International Workshop on Charge Transport and Excited State Processes in Organic Materials University College London, (2021); Electrochemical Society National Meeting, Chicago, IL, (2021); EMA2020, The American Ceramic Society, Orlando, FL (2020); 257th ACS National Meeting, Orlando, FL (2019); MRS Fall Meeting, Boston, MA (2018); 256th ACS National Meeting, Boston, MA, (2018); 2nd International Symposium of Molecular Design for Optoelectronic Materials, Beijing, China (2018); 254th ACS National Meeting, Washington DC (2017); SPIE, San Diego (2017); NT17, Belo Horizonte, Brazil (2017); CECAM, Bremen, Germany (2016); 252th ACS National Meeting, Philadelphia (2016); Gordon Conference, Barga, Italy (2016); 251th ACS National Meeting, San Diego (2016); PacificChem, Honolulu, (2015); Optical Probes, Hong Kong, (2015); 249th ACS National Meeting, Denver (2015); 55th Sanibel Symposium, St. Simons (2015); MRS Fall Meeting, Boston (2014); APS March Meeting, Denver (2014); MRS Fall Meeting, Boston (2013); Optical probes (OP-2013), Durham, UK (2013); 22nd I-APS meeting, Sarasota, FL (2013), 243th ACS National Meeting, San Diego, CA (2012), 242th ACS National Meeting, Denver, CO (2011), PacificChem, Honolulu HI (2010); CCTCC-19, Jackson, MS, (2010); CECAM, Ireland, (2010); Telluride Workshops, CO (2009-2016).

Selected publications (out of over 300):

Citation index over 20,000 (over 25,000), H-index 69 (76) according to Web of Science (Google Scholar)

- 1 R. Zubatyuk, B. Nebgen, J. S. Smith, S. Tretiak and O. Isayev, "Teaching neural network to attach and detach electrons from molecules" Nature Communication **12**, 4870 (2021).
- 2 M. Kulichenko, J. S. Smith, B. Nebgen, N. Fedik, A. I. Boldyrev, N. Lubbers, K. Barros and S. Tretiak, "The rise of neural networks for materials and chemical dynamics," Journal of Physical Chemistry Letters (Review, journal cover page) **12**, 6227 (2021).
- 3 V. M. Freixas, A. J. White, T. Nelson, H. Song, D. V. Makhov, D. Shalashilin, S. Fernandez-Alberti and S. Tretiak, "Non-Adiabatic Excited State Molecular Dynamics Methodologies: Comparison and Convergence," Journal of Physical Chemistry Letters (Review, journal cover page) **12**, 2970 (2021).

- 4 A. De Sio, E. Sommer, X. T. Nguyen, L. Gross, D. Popović, B. Nebgen, S. Fernandez-Alberti, S. Pittalis, C. A. Rozzi, E. Molinari, E. Mena-Osteritz, P. Bäuerle, T. Frauenheim, S. Tretiak, and C. Lienau, "Intermolecular conical intersections in molecular aggregates" Nature Nanotechnology, **16**, 63 (2021).
- 5 D. Ghosh, E. Welch, A. Neukirch, A. Zakhidov and S. Tretiak, "Polarons in Halide Perovskites: A Perspective" Journal of Physical Chemistry Letters (Review, journal cover page) **11**, 3271 (2020).
- 6 T. Nelson, A. White, J. Bjorgaard, A. Sifain, Y. Zhang, B. Nebgen, S. Fernandez-Alberti, D. Mozyrsky, A. Roitberg and S. Tretiak, "Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials" Chemical Reviews **120**, 2215 (2020).
- 7 B. J. Gifford, S. Kilina, A. Saha, X. He, Y. Kim, H. Htoon, S. K. Doorn and S. Tretiak, "Controlling Defect-State Emission in Covalently Functionalized Single-Walled Carbon Nanotubes" Accounts on Chemical Research, **53**, 1791 – 1801 (2020)
- 8 J. S. Smith, B. T. Nebgen, R. Zubatyuk, N. Lubbers, C. Devereux, K. Barros, S. Tretiak, O. Isayev, and A. E. Roitberg, "Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning" Nature Communications, **10**, 2903 (2019).
- 9 A. Saha, B. J. Gifford, X. He, G. Ao, M. Zheng, H. Kataura, H. Htoon, S. Kilina, S. Tretiak, S. K. Doorn "Chemical Selection of Emission State Configuration in a Quantum Light Emitter" Nature Chemistry **10**, 1089 (2018).
- 10 T. R. Nelson, D. Ondarse-Alvarez, N. Oldani, B. Rodriguez-Hernandez, L. Alfonso-Hernandez, J. F. Galindo, V.D. Kleiman, S. Fernandez-Alberti, A. E. Roitberg, S. Tretiak, "Coherent Exciton-Vibrational Dynamics and Energy Transfer in Conjugated Organics" Nature Communications, **9**, 2316 (2018).
- 11 H. Tsai, R. Asadpour, J.-C. Blancon, C. C. Stoumpos, O. Durand, J. W. Strzalka, B. Chen, R. Verduzco, P. M. Ajayan, S. Tretiak, J. Even, M. A. Alam, M. G. Kanatzidis, W. Nie, A. D. Mohite, "Light-induced lattice expansion leads to high-efficiency perovskite solar cells", Science, **360**, 67 (2018).
- 12 J.-C. Blancon, H. Tsai, W. Nie, C. C. Stoumpos, L. Pedesseau, C. Katan, M. Kepenekian, K. Appavoo, M. Y. Sfeir, S. Tretiak, M. G. Kanatzidis, J. Even, J. J. Crochet, A. D. Mohite, "Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites", Science, **355**, 1288 (2017).
- 13 H. Tsai, W. Nie, J.-C. Blancon, C.C. Stoumpos, R. Verduzco, B. Harutyunyan, S. Tretiak, L. Pedesseau, J. Even, M.A. Alam, G. Gupta, J. Lou, P.M. Ajayan, M.J. Bedzyk, M.G. Kanatzidis and A.D. Mohite "High-efficiency two-dimensional Ruddlesden-Popper perovskite solar cells", Nature, **536**, 312 (2016).
- 14 S. Kilina, D. Kilin and S. Tretiak, "Light-Driven and Phonon-Assisted Dynamics in Organic and Semiconductor Nanostructures," Chemical Reviews, **115**, 5929 (2015).
- 15 W. Nie, T. Hsinhan, R. Asadpour, J.C. Blancon, R. Kappera, M. Chhowalla, A. Neukirch, S. Tretiak, G. Gupta, J. Crochet, M.A. Alam, H.-L. Wang and A.D. Mohite, "High-efficiency solution-processed perovskite solar cells with millimeter-scale grains", Science, **347**, 522 (2015).
- 16 A. Zhugayevych and S. Tretiak, "Theoretical Description of Structural and Electronic Properties of Organic Photovoltaic Materials", Annual Reviews of Physical Chemistry, **66**, 306 (2015).
- 17 T. Nelson, S. F. Alberti, A. Roitberg, and S. Tretiak, "Excited-State Molecular Dynamics: Photophysics in Organic Conjugated Materials", Accounts on Chemical Research, **47**, 1155 (2014).
- 18 V. N. Gorshkov, S. Tretiak, and D. Mozyrsky, "Semiclassical Monte-Carlo approach for modeling non-adiabatic dynamics in extended molecules", Nature Communications, **4**, 2114 (2013).
- 19 J. Clark, T. Nelson, S. Tretiak, G. Cirmi, and G. Lanzani, "Femtosecond Torsional Relaxation", Nature Physics, **8**, 225-231 (2012).
Featured in: News & Views, Nature Physics **8**, 179 (2012) "A lightning-fast change".
- 20 S. Kilina, S. Ivanov, S. Tretiak, "Effect of surface ligands on optical and electronic spectra of semiconductor nanoclusters", Journal of the American Chemical Society, **131**, 7717 (2009).
- 21 F. Terenziani, C. Katan, M. Blanchard-Desce, E. Badaeva, and S. Tretiak, "Enhanced two-photon absorption of organic chromophores: theoretical and experimental assessments", Advanced Materials (Review Article, journal cover page) **20** 1-38 (2008).
- 22 S. Tretiak, "Triplet absorption in carbon nanotubes: a TD-DFT study", Nano Letters (journal cover page), **7**, 2201-2206 (2007).