Sergei Tretiak

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Professional employment history:

2017 – Present	Deputy Group Leader at T-1, Theoretical Division, LANL
2001 – Present	Technical Staff Member, Theoretical Division, LANL (currently Scientist 6)
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
1999 – 1999	Postdoctoral Associate, University of Rochester (Rochester, NY)
1994 – 1998	Graduate Student, University of Rochester (Rochester, NY)
1991 – 1994	Graduate Student, Institute of Spectroscopy of Russian Academy of Sciences
1987 – 1991	Undergraduate Student, Moscow Institute of Physics and Technology, Russia

Academic background:

1999 Ph.D. in Chemistry, University of Rochester (Rochester, NY),
Advisor: Professor Shaul Mukamel. Thesis title: *"Collective Electronic Excitations in Spectroscopy of Conjugated and Aggregated Molecules"*;

1994 M.S. in Chemistry, Department of Chemistry, University of Rochester (Rochester, NY);

1994 M.S. in Physics (Highest Honors), Institute of Physics and Technology (Moscow, Russia)

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.

Program Development at LANL:

- PI/co-PI of five LDRD-DR (Laboratory Directed Research and Development-Directed Research) projects;
- PI of seven LDRD-ER (Exploratory Research) projects;
- Co-Inv of multiple LDRD, NSF, DOE-OBES and EFRC projects;

- Helped to establish LANL theory programs on excited states, spectroscopy and dynamics of conjugated polymers, organic chromophores, carbon nanotubes, mixed halide perovskites and semiconductor nanoparticles, as well as machine learning for materials science.

Professional Awards and Honors:

- 'Ioannidis list' of top 2% cited scientists (2020), Stanford, https://data.mendeley.com/datasets/btchxktzyw/2;
- Sci. Adv. **6**, eaay0815 (2020) was chosen by Physics World editorial team as one of its "Top 10 Breakthroughs of the Year." https://physicsworld.com/a/physics-world-announces-its-breakthrough-of-the-year-finalists-for-2020/
- Fellow of the Royal Society of Chemistry, FRSC (2019), UK;
- The 2019 Highly Cited Researchers list from the Web of Science Group;
- Laboratory Fellow (2018), Los Alamos National Laboratory, US;
- Visiting Lecturer at CRC Center (2018), University of Heidelberg, Germany;
- LANL Postdoctoral Distinguished Mentor (2015), Los Alamos National Laboratory, US;
- APS Fellow (2014), Division of Chemical Physics, American Physical Society, US;
- LANL Fellows Prize (2010), Los Alamos National Laboratory, US;
- Invited Lecturer, Winter School in Theoretical Chemistry on Nanophotonics (2005), University of Helsinki, Finland;
- Slansky Fellow Award (2001), Los Alamos National Laboratory, US;
- LANL Director's Postdoctoral Fellow (1999-2001), Los Alamos National Laboratory, US;
- Arnold Weissberger Fellow (1997-1998), University of Rochester, US;
- ACS Graduate Student Award in Computational Chemistry (1996), Division of Physical Chemistry, American Chemical Society, US;
- Elon Huntington Fellow (1996-1997), University of Rochester, US;
- Sherman Clarke Fellow (1996-1997), University of Rochester, US;
- Diploma with Honor ["Red Diploma"] (1994), Moscow Institute Physics and Technology;
- Special Institute Fellowship (1992-1994), Moscow Institute of Physics and Technology, Russia.

Highlights of professional service at LANL:

- 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 virtual conferences at CNLS, LANL: *"Machine Learning in Chemical and Materials Sciences"*, Los Alamos, NM, May 2021.
- Co-organizer of the virtual Quantum Science Workshop at LANL, April 2021.
- Member of LDRD ER Refresh Committee, LANL, 2020.
- Co-organizer of the conferences at CNLS, LANL: *"Physics Informed Machine Learning"*, Santa Fe, NM, 2016 and 2018.
- Co-organizer of the 29th CNLS Annual Conference *"Energy for the 21th century"*, Santa Fe, NM, 2009.
- Co-organizer of the 27th CNLS Annual Conference *"Complexity of Biological and Soft Materials"*, Santa Fe, NM, 2007.

- Organizer of the conference at CNLS, LANL: *"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, 2006-2009.
- Co-lead (with S. K. Doorn) Integrated Nanomaterials Area of Leadership (AoL) in Materials for the Future Pillar (2018-2019).
- Member Quantum Information Science (QIS) S&T working group at LANL (2019-present).
- Member of CNLS Executive Committee, LANL, 2004-present.
- Member of CNLS public service committee, Los Alamos National Laboratory, 2001-2003.
- Manager of the Center for Integrated Nanotechnologies (CINT) Colloquium series, LANL/SNL, 2009-2012.
- Manager of the Theoretical Division P/T Colloquium series, LANL, 2001-2005.
- Member of LANL LDRD-DR science review committee in Information Science and Technology, SAP IS&T, 2018-present.
- Member of LANL LDRD-ER review committee in Quantum and Optical Science, 2007, 2012, 2012, 2013.
- Member of LANL LDRD-ER review committee in Chemistry and Materials category, 2005.
- Member of LANL LDRD-ER review committee in Technology category, 2004.

Highlights of professional service elsewhere:

- Organizer of the focused session *"Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters"* for the International Pacifichem conference, Honolulu, Hawaii, December 2015, December 2022.
- Organizer of Telluride workshop series *"Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy"*, Telluride, CO, 2007, 2009, 2011, 2013, 2015, 2017, 2019, 2021.
- Co-organizer of the Telluride workshop series: *"Machine Learning and Informatics for Chemistry and Materials"*, Telluride, CO, 2018, 2019, 2021.
- Member of Executive Committee for Virtual International Seminar on Theoretical Advancements (VISTA), 2020-present.
- Member of NSF Chemistry Division Committee of Visitors (COV), May 2020.
- Organizer of the Inaugural Symposium for "*Computational Materials Program of Excellence*", Skolkovo Institute of Science and Technology (SkolTech), Moscow, Russia, September 2019.
- Co-organizer of the Telluride workshop series: *"Electronic and Structural Dynamics in Hybrid Perovskites: Theory Meets Experiment"*, Telluride, CO, 2016, 2018.
- Co-organizer of the session *"Physical Chemistry of Interfaces and Nanomaterials"* for the SPIE Nano Science and Engineering conference, San Diego, CA, 2007, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2020, 2021, 2022.
- Co-organizer of the Telluride workshop: *"Non-Equilibrium Statistical Physics: from molecular materials to theoretical engineering. Honoring Professor Vladimir Chernyak 60th Birthday"*, Telluride, CO, 2016.

- Co-organizer Multidisciplinary Program Planning Group on *"Computational Materials and Nanoscience: Theory meets experiment"*, the 251st ACS National Meeting, San Diego, CA, March 2016.
- Co-organizer of the focused symposium *"Frontiers in Solar Light Harvesting Processes"*, 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.
- Organizer of the session *"Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters"* for the International Pacifichem 2015 conference, Honolulu, Hawaii, December 2015.
- Co-organizer of the International Conference on *"Organic Solar Cells: Theory and Experiment, From Description to Prediction"* (OPV-2013), Santa Fe, NM, May 2013.
- Organizer of the 9th International Conference on *"Optical Probes of Conjugated Polymers and Organic Nanostructures"* (OP-2011), Santa Fe, NM, June 2011.
- Co-organizer of the APS Focus Session: *"Electronic Structure and Applications to Energy Conversion"*, for the APS March Meeting, Dallas, TX, 2011.
- Co-organizer of the Conference *"Life in Liouville Space: 30 Years of Theoretical Spectroscopy"*, Irvine, CA, 2008.
- Member of the International Advisory Board of conference series on Optical Probes of Conjugated Polymers and Organic Nanostructures (2011-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 (2016-2018).
- Member of Editorial Board of Advances in Physical Chemistry (2011-2018);
- Member of Journal of Physical Chemistry Letters Editorial Advisory Board (2018-present);
- Affiliations ACS/APS/MRS/OSA/ECS/AAAS/RSC.

Mentor of 31 Postdocs (2001-present):

- Artem Masunov, 2001-2004, now faculty at the University of Central Florida;
- Rudolph Magyar, 2003-2005, now staff scientist at Northrop Grumman;
- Andrei Piryatinski, 2002-2006, now staff scientist (T-4) at LANL;
- Sergei Goupalov, 2003-2004, now faculty at Jackson State University;
- Melissa Lucero, 2005-2006, now Chief Scientist, Theory & Synthesis MLucero Consulting;
- Michael Galperin (Director Fellow), 2007-2008, now faculty at the UC San Diego;
- Jianmin Tao (Director Fellow), 2007-2010, now faculty at Tulane University;
- Svetlana Kilina (Director Fellow), 2008-2010, now faculty at North Dakota State Univ.;
- Kirill Velizhanin, 2010-2012, now staff scientist (T-1) at LANL;
- Hao Li, 2011-2014, now postdoc at the University of Houston;
- Andriy Zhugayevych, 2011-2014, now faculty at Skoltech, Moscow, Russia;
- Alexei Roslyak, 2012-2014, now faculty at Fordham University;

- Tammie Nelson, Feynman Fellow, 2013-2016, now staff scientist (T-1) at LANL;
- Ludmila Adamska, 2013-2016, now postdoc at Padova University;
- Josiah Bjorgaard, 2013-2016, now Materials Scientist at TerraPower LLC, Seattle;
- Alexander White, 2014-2017, now staff scientist (T-1) at LANL;
- Amanda Neukirch (Director Fellow), 2014-2017, now staff scientist (T-1) at LANL;
- Benjamin Nebgen, 2016-2018, now staff scientist (T-1) at LANL;
- Liujiang Zhou (Director Fellow), 2017-2019, now faculty at UESTC, Chengdu, China;
- Yu Zhang (Director Fellow), 2018-2019, now staff scientist (T-1) at LANL;
- Brendan Gifford, 2018-2019, now staff scientist (T-1) at LANL;
- Justin Smith (Metropolis Fellow), 2018-2020, now staff scientist (T-1) at LANL;
- Hsinhan (David) Tsai (Oppenheimer Fellow), 2019-2020, now First Solar, USA;
- Dan Liu, 2020-2020, now faculty at Southeast University, China
- Galen Craven (Director Fellow), 2019-2020, now staff scientist (T-1) at LANL;
- Dibyajyoti Ghosh, 2018-2021, now faculty at IIT Delhi, India;
- Walter Malone, 2019-2021, now faculty at Tuskegee University, AL;
- Huajing (Wilson) Song, 2019-present;
- Guoqing Zhou, 2021-present;
- Ashutosh Kumar, 2021-present;
- Adela Habib, 2021-present.

Mentor of over 100 (under) graduate students (UGS/GRA) at CNLS/CINT/LANL

Current collaborations:

- ***Within LANL:*** A. Saxena, A.R. Bishop, W. Nie, S.K. Doorn, H. Htoon, S.D. McGrain, J. Hollingsworth, K. Barros, N. Lubbers, J. Smith, B. Nebgen, A. Piryatinski, D. Mozyrsky, V. Klimov, P. Dub, L. Cincio, S. Mniszewski, Y. Zhang.
- ***Outside LANL****:* S. Mukamel (UCI), G. C. Bazan (UCSB), J. Martinez (ASU), A. Mohite (Rice), T. Frauenheim (Bremen, Germany), C. Lienau (Oldenburg, Germany), A. de Silo (Oldenburg, Germany), J. Lupton (Regensburg, Germany), V. Chernyak (Wayne State U.), J. Even (Rennes, France), C. Katan (Rennes, France), D. Shalashilin (Leeds, UK), O. Prezhdo (USC), G. Lanzani (Italy), T.-Q. Nguyen (UCSB), S. Kilina (NDSU), D. Kilin (NDSU), S. Fernandez-Alberti (Argentina), A. Roitberg (U. Florida), O. Isayev (UNC), Y. Zhao (NTU, Singapore), A. Zhugayevych (Skoltech, Russia), H. L. Wang (SUST, China).

Record of support:

- LANL LDRD ER*"Excited state molecular dynamics of large molecules"* (2001-2004, $250k/year) Role: PI
- LANL LDRD DR*"Electronic interactions on nanometer lengthscales"* (2000-2003) Role: co-I
- OBES "*Molecularly Engineered Biomimetic Nano-assemblies"* (2003-2007) Role: co-I
- OBES "*Multiparticle and Interfacial Interactions in Nanoscale Systems Built from Nanocrystal Quantum Dots"* (2003-2006) Role: co-I

- US Army *"Quantum computation using self-assembled molecular spin arrays"* (2002-2005) Role: co-I
- LANL LDRD DR*"Interfacial Energy and Charge Transfer in Multifunctional Bio-Inspired Nano-Assemblies"* (2003-2006) Role: co-I
- DOE Center for Integrated Nanotechnologies (CINT) (2005-present, $230/year) Role: Staff Scientist
- DOE/BES funded Next Generation Lighting Initiative (2005-2012) Role: co-I
- LANL LDRD ER*"Excited states and optical response of nanosized molecules at linear scaling numerical cost"* (2007-2009, $300k/year) Role: PI
- LANL LDRD ER*"Photodynamics and photochemistry of carbon nanotube materials"* (2009-2011, $300k/year) Role: PI
- DOE EFRC *"Center of Advanced Solar Photophysics"* CASP (2011-2014, $150k/year) Role: Theory PI
- DOE EFRC *"Center for Energy Efficient Materials"* CEEM (2011-2014, $120k/year) Role: LANL team PI
- LANL LDRD ER*"Quasiparticle Scattering for Multiscale Modeling of Electronic Materials"* (2011-2013, $300k/year) Role: PI
- LANL LDRD DR*"Organic Electronic Materials: Designing and Creating Functional Interfaces"* (2012-2014, $1,900/year) Role: PI
- LANL LDRD DR*"Fighting Carbon with Carbon: All-Carbon Nanomaterial Photovoltaics"* (2013-2015) Role: co-I
- LANL LDRD ER*"Excited State Quantum Interactions in Carbon Nanotubes"* (2013-2015) Role: co-I
- LANL LDRD DR*"Photoactive Energetic Materials for Quantum Optical Initiation"* (2014-2016, $1,900/year) Role: co-PI
- LANL LDRD ER*"Perovskite solar cells: the next frontier in energy harvesting"* (2015-2017) Role: co-I
- LANL LDRD ER*"Computational algorithms for modeling non-adiabatic dynamics in molecular systems"* (2017-2019) Role: co-I
- LANL LDRD ER*"Harnessing Dark Excitons in Carbon Nanotubes through Covalent Doping Chemistry"* (2017-2019) Role: co-I
- LANL LDRD DR*"Hybrid Photonic-Plasmonic Materials: Toward Ultimate Control Over the Generation and Fate of Photons"* (2017-2019) Role: co-I
- DOE OBES *"Understanding Novel Lewis Acid Doping Mechanisms in Organic Semiconductors"* (2018-2020), UCSB centered. Role: Theory PI
- NSF DMREF *"Metallic-type transport in polymers: Establishing materials design criteria and predicting structure/property interrelations"* (2018-2020), GaTech centered. Role: co-I
- LANL LDRD ER *"Hamiltonian on Demand for Computational Materials Using Machine Learning"* (2018-2020, $320k/year) Role: PI
- LANL LDRD DR *"Rational Design of Hybrid Perovskites for Next Generation Gamma-ray Detection"* (2018-2020, $1,700k/year) Role: PI

- DOE BES "*Theory and Simulation of Ultrafast Multidimensional Nonlinear X-ray Spectroscopy of Molecules"* (2018-2021, $175k/year) Role: LANL PI
- LANL LDRD DR *"Quantum Photonics with Semiconductor Nanocrystals"* (2020-2022, $1,700k/year) Role: co-PI
- LANL LDRD DR *"Quantum Chemistry using Quantum Computers"* (2020-2022) Role:co-I
- LANL LDRD DR *"Data Driven Modeling of Non-Equilibrium Dynamics in Chemical and Materials Systems"* (2021-2023, $1,700k/year) Role: co-PI
- LANL LDRD DR *"Accelerating Nuclear Fuel Qualification through Integrated Multiscale and Multiphysics Models"* (2022-2024, $1,700k/year) Role: co-I
- DOE BES "*Modeling of Multidimensional X-ray Probes of Chemical Processes and Dynamics in Molecular Systems"* (2022-2024, $175k/year) Role: LANL PI
- DOE BES "*Data science driven quantum chemistry for reactive chemistry controlled by stimuli"* (2022-2024, $800k/year) Role: co-PI

Refereeing for Journals (typical):

Proceedings of the National Academy of Science	Physical Review A, B, C
International Journal of Quantum Chemistry	Physics Review Letters
Journal of the American Chemical Society	Applied Physics Letters
Journal of Chemical Theory and Computation	Chemical Physics Letters
Journal of Physical Chemistry A, B, C	Chemical Physics
Journal of Physical Chemistry Letters	ACS Nano
New Journal of Physics	Nano Letters
Physical Chemistry Chemical Physics	Energy Letters
Journal of Luminescence	Physics Letters A
Journal of Chemical Physics	Macromolecules
Scientific Reports	Physica B, D
Advanced Science	RSC Advances
Advanced Functional Materials	Science Advances
Computational Materials Science	Science
Nature Communications	Nature
Nature Materials	Nature Physics

Refereeing for Agencies (typical):

National Science Foundation (NSF)	NSF Centers
Petroleum Research Fund (PRF-ACS)	US Air Force AFMC AFOSR
US Department of State for the Science Centers	US Army Research Office
Office of Basic Energy Sciences (OBES) at DOE	US Navy Research Office
John D. and Catherine T. MacArthur Foundation	US BES Nanocenters
Research Corporation Award Programs	Austrian Science Fund (FWF)
Natural Sciences & Engineering Research Council, Ca	National Research Foundation, Singapore
Netherlands Foundation for Fundamental Research	European Research Council (ERC)

Laboratory-Directed Research and Development	Russian Foundation for Basic Research
Swiss National Science Foundation	Israel Science Foundation
French National Research Agency (ANR)	Czech National Science Foundation
The Science and Technology Center in Ukraine	Croatian Science Foundation
Habilitation Promotion Faculty Reviewer (Europe and UK)	Tenure Promotion Faculty Reviewer (US, Canada, Israel, Brazil, Mexico, Russia)

Professional References:

Name/address	*Name/address*
Professor Guillermo C. Bazan Department of Chemistry National University of Singapore Singapore 117543 E-mail: chmbgc@nus.edu.sg (65)-6601-2009 (phone)	**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)
Professor Jean-Luc Brédas Department of Chemistry and Biochemistry University of Arizona Tucson, Arizona 85721-0041 E-mail: jlbredas@arizona.edu (520) 626-7103 (phone)	**Professor Sir Richard Friend** Cavendish Laboratory JJ Thomson Avenue Cambridge CB3 0HE E-mail: rhf10@cam.ac.uk +44 (0)1223 337218 (phone)
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Invited/keynote talks (over 300) and other presentations

- *"The rise of neural networks for materials and chemical dynamics"* (invited seminar), Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, October 2021.
- *"In the quest for excited states: from machine learning to non-adiabatic dynamics"* (invited talk), Wintergreen Meeting of Physical Chemists, Wintergreen, VA, September 2021.
- *"Modeling of charge dynamics in hybrid perovskites"* (invited talk), ACS National Fall Meeting, Atlanta, GA, August 2021.
- *"From NAMD method comparisons to modeling of coherent photoexcited dynamics"* (invited talk), Virtual Telluride Workshop on Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, July 2021.
- *"Transient (De) Localization in Molecular Coherent Energy Transfer"* (invited talk), International Workshop on Charge Transport and Excited State Processes in Organic Materials University College London, June 2021.
- *"Photoexcited dynamics in molecular materials with Non-adiabatic EXcited state Molecular Dynamics (NEXMD) code"* (invited tutorial lecture), Virtual CyberTraining Workshop, Buffalo University, Buffalo, NY, June 2021.
- *"Coherent Photoexcited Dynamics in Molecular systems"* (invited talk), Virtual Telluride Workshop on Spatio-Temporal Dynamics of Excitons, Telluride, CO, June 2021.
- *"Coherent Photoexcited Dynamics and Intermolecular Conical Intersections"* (invited virtual colloquium), Julius-Maximilians-Universität Würzburg, Würzburg, Germany, June 2021.
- *"Coupling between Quantum Defects in Carbon Nanotubes"* (invited virtual talk), Electrochemical Society National Meeting, Chicago, IL, June 2021.
- *"Carbon Nanotubes and Semiconductor Nanocrystals for Quantum Photonics"* (invited virtual talk), Quantum Science Workshop at LANL, Los Alamos, NM, April 2021.
- *"Coherent Photoexcited Dynamics and Intermolecular Conical Intersections"* (invited virtual talk), Quantum Dynamics of Excitons and Exciton-Light Interactions Virtual Mini-conference Series, City University of New York, NY, March 2021.
- *"Coherent Photoexcited Dynamics and Intermolecular Conical Intersections"* (invited virtual colloquium), Center for Non-Linear Studies (CNLS), LANL, Los Alamos, NM, December 2020.
- *"Coherent Photoexcited Dynamics and Intermolecular Conical Intersections"* (invited virtual keynote talk), Materials Research Society (MRS) Fall Meeting, Boston, MA, December 2020.
- *"Coherent Photoexcited Dynamics and Intermolecular Conical Intersections"* (invited virtual seminar), VISTA Seminar Series, University at Buffalo, SUNY, Buffalo, NY, November 2020.
- *"Machine Learning for Molecular Properties and Materials"* (invited virtual seminar), MateriAlz Virtual Seminar Series, Arizona State University, Tucson, AZ, October 2020.

- *"Hybrid 2D and 3D Nanostructured Perovskites: From Understanding Fundamental Physics to Optoelectronic Applications"* (invited virtual lecture), Tnano20: Virtual International Workshop on Nanotechnology, Tbilisi, Republic of Georgia, October 2020.
- *"Machine Learning for Molecular Properties and Materials"* (invited seminar), Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, February 2020.
- *"Machine Learning for Chemistry and Materials"* (invited talk), Electronic Materials and Applications 2020 (EMA 2020) conference, The American Ceramic Society, Orlando, January 2020.
- *"Halide Perovskites—From Understanding Fundamental Physics to Optoelectronic Applications"* (invited talk), Materials Research Society (MRS) Fall Meeting, Boston, MA, December 2019.
- *"Machine Learning for Chemistry and Materials"* (invited seminar), University of California, Irvine (UCI), Irvine, November 2019.
- *"Machine Learning for Chemistry and Materials"* (invited seminar), Goethe-Universitaet, Frankfurt, Germany, October 2019.
- *"Machine Learning for Chemistry and Materials"* (invited seminar), Université de Rennes, Rennes, France, October 2019. .
- *"From multiple cloning to polaritonics in excited state molecular dynamics"* (invited talk) CECAM Workshop "Thinking outside the box" Bremen, Germany, October 2019.
- *"Extended Hückel theory resurrected: dynamic parameterization of effective Hamiltonians using deep learning"* (invited talk) CECAM Workshop "Thinking outside the box" Bremen, Germany, October 2019.
- *"Machine Learning for Chemistry and Materials"* (invited talk) at Center for Integrated nanotechnology (CINT) Annual Meeting, Santa Fe, NM, September 2019.
- *"Modeling of Electronic Properties in Organic and Hybrid Materials"* (invited tutorial lecture) at 5th International Fall School on Organic Electronics (IFSOE-2019), Moscow, Russia, September 2019.
- "*Hybrid Perovskite: From Understanding Fundamental Physics to Optoelectronic Applications"* (invited colloquium), Skolkovo Institute of Science and Technology (SkolTech), Moscow, Russia, September 2019.
- *"Machine Learning for Molecular Properties and Materials"* (tutorial talk) at CMP Inaugural Symposium, Skolkovo Institute of Science and Technology (SkolTech), Moscow, Russia, September 2019.
- *"Machine Learning for Molecular Properties and Materials"* (invited seminar), Department of Chemistry and Biochemistry, GaTech, Atlanta, GA, August 2019.
- *"Hybrid Perovskite: From Understanding Fundamental Physics to Optoelectronic Applications"* (invited talk), Nanomaterials: Computation, Theory, and Experiment, Telluride, CO, July 2019.
- *"Multiple cloning and polaritons in excited state non-adiabatic molecular dynamics"* (invited talk), Telluride Workshop on Non-Equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, July 2019.
- *"Hybrid Perovskite: From Understanding Fundamental Physics to Optoelectronic Applications"* (keynote lecture), Photovoltaic Summer Workshop, Academia Sinica, Taipei, Taiwan, July 2019.

- *"Machine Learning for Molecular Properties and Chemistry"* (invited seminar), Research Center for Applied Science, Academia Sinica, Taipei, Taiwan, July 2019.
- *"From coherences to polaritons in excited state non-adiabatic molecular dynamics"* (invited talk), Telluride Workshop on Quantum Dynamics and Spectroscopy in Condensed-Phase Materials and Bio-Systems, Telluride, CO, June 2019.
- *"Exciton-phonon dynamics in conjugated light harvesters and hybrid perovskites"* (invited talk), Wintergreen Meeting of Physical Chemists, Wintergreen, VA, June, 2019.
- *"Modeling Insights into Optical Properties of Functionalized Carbon Nanotubes"* (invited talk), Electrochemical Society National Meeting, Dallas, TX, May 2019.
- *"Machine Learning for Molecular Properties and Chemistry"* (invited graduate student seminar), UCSB, Santa Barbara, CA, May 2019.
- *"Exciton-phonon dynamics in conjugated light harvesters and hybrid perovskites"* (invited physchem seminar), UCSB, Santa Barbara, CA, May 2019.
- *"Machine Learning for Molecular Properties and Chemistry"* (invited seminar), topical DMREF project meeting, GaTech, Atlanta, GA, May 2019.
- *"Machine Learning for Molecular Properties and Chemistry"* (invited talk), IMS workshop on Computational Data Science Approaches for Materials, LANL, Los Alamos, NM, April 2019.
- *"Simulation of photoexcited dynamics in large molecules"* (invited talk), 257th ACS National Meeting, Orlando, FL, April 2019.
- *"Machine Learning for Molecular Properties and Chemistry"* (invited talk), 257th ACS National Meeting, Orlando, FL, April 2019.
- *"Chemical functionalization and optical properties of carbon nanotube materials"* (invited seminar), Department of Mechanical & Aerospace Engineering, NMSU, Las Cruces, NM, March 2019.
- *"Hybrid Perovskite: From Understanding Fundamental Physics to Optoelectronic Applications"* (invited seminar), Department of Chemistry, Brandeis University, March 2019.
- *"Machine Learning for Molecular Properties and Chemistry"* (invited MSE-colloquium), Nanyang Technological University, Singapore, March 2019.
- *"Machine Learning for Molecular Properties and Chemistry"* (invited lecture), Institute for Molecular Science, Okazaki, Japan, February 2019.
- *"Machine Learning for Molecular Properties and Chemistry"* (invited lecture), Kyoto University, Kyoto, Japan, February 2019.
- *"Coherent Exciton-Vibrational Dynamics and Energy Transfer in Conjugated Chromophores"* (invited talk), Materials Research Society (MRS) Fall Meeting, Boston, MA, December 2018.
- *"Hybrid Perovskite: From Understanding Fundamental Physics to Optoelectronic Applications"* (invited seminar), Department of Chemistry, UC Berkeley, November 2018.
- *"Machine Learning for Molecular Properties and Chemistry"* (invited seminar), Moscow Institute of Physics and Technology (MIPT), Dolgoprudny, Russia, November 2018.
- "*Hybrid Perovskite: From Understanding Fundamental Physics to Optoelectronic Applications"* (invited colloquium), Skolkovo Institute of Science and Technology (SkolTech), Moscow, Russia, November 2018.

- *"Simulation of photoexcited dynamics in molecules",* (invited colloquium), Center for Non-Linear Studies (CNLS), LANL, Los Alamos, NM, October 2018.
- *"Machine Learning for Molecular Properties"*, (invited talk), Telluride Workshop on Machine Learning and Informatics for Chemistry and Materials, Telluride, CO, October 2018.
- *"The NEXMD computational framework for nonadiabatic excited state dynamics in large molecules"* (invited talk), The 10th International Meeting on Photodynamics and Related Aspects (IMPRA), Cartagena, Columbia, September 2018.
- *"Machine Learning for Molecular Properties"*, (invited talk), Universidad de los Andes, Bogota, Columbia, September 2018.
- *"Machine Learning for Molecular Properties"*, (invited talk), Universidad Nacional de Colombia, Bogota, Columbia, August 2018.
- *"Coherence and energy transfer in conjugated chromophores"* (invited talk), 256th ACS National Meeting, Boston, MA, August 2018.
- *"Advances and Promises of Layered Hybrid Perovskite Semiconductors"* (invited talk), 256th ACS National Meeting, Boston, MA, August 2018.
- *"The NEXMD computational framework for nonadiabatic excited state dynamics in large molecules"* (invited talk), Telluride Workshop on Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems, Telluride, CO, July 2018.
- *"Coherent Exciton-Vibrational Dynamics and Energy Transfer in Conjugated Organics"* (invited talk), Telluride Workshop on Electronic and Structural Dynamics in Hybrid Perovskites: Theory Meets Experiment, Telluride, CO, July 2018.
- *"Efficient non-adiabatic excited state dynamics simulations in extended molecular system"* (invited talk), MolSSI workshop, the University at Buffalo, Buffalo, June 2018.
- *"Coherent exciton-vibrational dynamics and energy transfer in conjugated organics"* (invited seminar), Department of Chemistry, Tsinghua University, April 2018.
- *"Advances and Promises of Layered Hybrid Perovskite Semiconductors"* (invited seminar), Department of Chemistry, Southern University of Science and Technology, Shenzhen, China, April 2018.
- *"Efficient non-adiabatic excited state dynamics simulations in extended molecular systems"* (keynote talk), the 2nd International Symposium of Molecular Design for Optoelectronic Materials, Beijing, China, April 2018.
- *"Coherent exciton-vibrational dynamics and energy transfer in conjugated organics"* (invited seminar), School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, March 2018.
- *"Efficient non-adiabatic excited state dynamics simulations in extended molecular systems"* (invited seminar), Department of Chemistry, University of Houston, Houston, March 2018.
- *"Chemical functionalization and optical properties of carbon nanotube materials"* (invited seminar), Department of Chemistry, Rice University, March 2018.
- *"Efficient non-adiabatic excited state dynamics simulations in extended molecular systems"* (invited colloquium), University of Bremen, Bremen, Germany, January 2018.
- *"Coherent exciton-vibrational dynamics and energy transfer in conjugated organics"* (invited colloquium), Department of Chemistry, University of Heidelberg, Heidelberg, Germany, February 2018.

- *"Chemical functionalization and optical properties of carbon nanotube materials"* (invited colloquium), Department of Chemistry, University of Heidelberg, Heidelberg, Germany, February 2018.
- *"Efficient non-adiabatic excited state dynamics simulations in extended molecular systems"* (invited colloquium), Department of Chemistry, University of Heidelberg, Heidelberg, Germany, January 2018.
- *"Advances and Promises of Layered Hybrid Perovskite Semiconductors"* (invited seminar), Department of Physics, Texas State University, San Marcos, TX, November 2017.
- *"Advances and Promises of Layered Hybrid Perovskite Semiconductors"* (invited seminar), Landau Institute for Theoretical Physics, Chernogolovka, Russia, November 2017.
- *"Coherent exciton-vibrational dynamics and energy transfer in conjugated organics"* (invited colloquium), Skolkovo Institute of Science and Technology (SkolTech), Moscow, Russia, November 2017.
- *"Coherent exciton-vibrational dynamics and energy transfer in conjugated organics"* (invited talk), CECAM Workshop on Charge carrier dynamics in nanostructures: optoelectronic and photo-stimulated processes, Bremen, Germany, October, 2017.
- *"Coherent exciton-vibrational dynamics and energy transfer in conjugated organics"* (invited talk), 254th ACS National Meeting, Washington, DC, August 2017.
- *"Intra- and inter-molecular energy transfer in organic semiconductors: insights from non-adiabatic dynamics simulations"* (invited talk), SPIE session on Physical Chemistry of Semiconductor Materials and Interfaces XVI, San Diego, CA, August 2017.
- *"Coherent Exciton-Vibrational Dynamics and Energy Transfer in Conjugated Organics"* (invited talk), Telluride Workshop on Spontaneous Coherence and Collective Dynamics, Telluride, CO, July 2017.
- *"Advances and Promises of Layered Halide Hybrid Perovskites, LANL updates"* (invited talk), Telluride Workshop on Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, July 2017.
- *"Advances and Promises of Layered Halide Hybrid Perovskites, LANL updates"* (invited talk), Telluride Workshop on Nanomaterials: Computation, Theory, and Experiment, Telluride, CO, July 2017.
- *"Chemical functionalization and optical properties of carbon nanotube materials"* (invited talk), Telluride Workshop on Defect Chemistry and Physics of Low Dimensional Materials, Telluride, CO, July 2017.
- *"Electronically excited states dynamics and theoretical spectroscopy"* (invited seminar), Universidad Nacional de Quilmes, Bernal, Argentina, June 2017.
- *"Chemical functionalization and optical properties of carbon nanotube materials"* (invited talk), 18th International Conference on the Science and Application of Nanotubes and Low - Dimensional Materials, Belo Horizonte, Brazil, June 2017.
- *"Advances and Promises of Layered Halide Hybrid Perovskites (LANL updates)"* (invited talk), 12th International Conference on Optical Probes of Organic and Hybrid Semiconductors (OP2017), Quebec City, Canada, June 2017.
- *"Modeling of photophysics and energy transfer in organic molecules"* (invited seminar), Moscow State University (MSU), Moscow, Russia, November 2016.

- *"Chemical functionalization and optical properties of carbon nanotube materials"* (invited seminar), Moscow Institute of Physics and Technology (MIPT), Dolgoprudny, Russia, November 2016.
- "*On the way toward efficient perovskite photovoltaics and beyond"* (invited colloquium), Skolkovo Institute of Science and Technology (SkolTech), Moscow, Russia, November 2016.
- *"On the way toward efficient perovskite photovoltaics and beyond"* (invited talk), the 72nd Annual ACS SouthWestern Regional Meeting, Galveston, TX, November 2016.
- "*Modeling of photophysics and energy transfer in large molecular systems"* (invited talk), the 72nd Annual ACS SouthWestern Regional Meeting, Galveston, TX, November 2016.
- *"On the way toward efficient perovskite photovoltaics and beyond"* (invited talk), CECAM Workshop on Computational insight into photo-induced processes at interfaces, Bremen, Germany, October 2016.
- *"A few lessons from non-adiabatic excited state dynamics simulations of large molecules"* (invited seminar), University de Rennes, Rennes, France, October 2016.
- *"Modeling of photophysics and energy transfer in organic semiconductors"* (invited talk), ZING conferences in Organic Semiconductors Dubrovnik, Croatia, September, 2016.
- *"On the way toward efficient perovskite photovoltaics and beyond"* (invited colloquium), Department of Chemistry, New Mexico Tech Socorro, NM, September, 2016.
- *"Theoretical insights into multiscale electronic processes in organic photovoltaics"* (invited talk), 252st ACS National Meeting, Philadelphia, CA, August 2016.
- *"On the way toward efficient perovskite photovoltaics and beyond"* (invited talk), LANL MaRIE workshop: High-energy and Ultrafast X-Ray Imaging Technologies and Applications, Santa Fe, NM, August 2016.
- *"Modeling of photophysics and energy transfer in molecular materials"* (invited talk), LANL MaRIE workshop: Probing Dynamic Processes in Soft Materials Using Advanced Light Sources, Santa Fe, NM, July 2016.
- *"On the way toward efficient perovskite photovoltaics and beyond"* (invited talk), Telluride Workshop on Charge and Energy Transfer in Photoreactions and Photodynamics, Telluride, CO, July 2016.
- *"Chemical functionalization and optical properties of carbon nanotube materials"* (invited talk), Telluride Workshop on Non-Equilibrium Statistical Physics: from molecular materials to theoretical engineering. Honoring Professor Vladimir Chernyak 60th Birthday, Telluride, CO, July 2016.
- *"Electronic processes in organic semiconductors: theory meets experiment"* (invited talk), Telluride Workshop on Electronic and Structural Dynamics in Hybrid Perovskites: Theory Meets Experiment, Telluride, CO, July 2016.
- *"Modeling of photophysics and energy transfer in organic semiconductors"* (invited talk), Gordon conference: Electronic Processes in Organic Materials, Barga, Italy, June 2016.
- *"On the way toward efficient perovskite photovoltaics and beyond"* (invited seminar), Istituto Italiano di Tecnologia (IIT), Center for Nanoscience and Technology, Milan, Italy, June 2016.
- *"Modeling of photophysics and energy transfer in organic semiconductors"* (invited seminar), Department of Pharmacy and Physical Chemistry, University of Barcelona, Barcelona, Spain, May 2016.

- *"Modeling of photophysics and energy transfer in organic semiconductors"* (invited seminar), Madrid Institute of Advanced Studies, IMDEA, Madrid, Spain, May 2016.
- *"Theoretical insights into multiscale electronic processes in organic photovoltaics"* (invited talk), 251st ACS National Meeting, San Diego, CA, March 2016.
- *"A few roadblocks on the way toward efficient perovskite photovoltaics"* (invited talk), 251st ACS National Meeting, San Diego, CA, March 2016.
- *"Our journey to the land of excited state dynamics in large molecules"* (invited talk), 251st ACS National Meeting, San Diego, CA, March 2016.
- *"A few lessons from non-adiabatic excited state dynamics simulations of large molecules"* (invited talk), Pittcon 2016: ABB- Bomem-Michelson Award symposium, Atlanta, GA, March 2016.
- *"A journey to the land of excited state dynamics in organic semiconductors"* (invited talk), 2016 Mesilla Chemistry Workshop on Electrochemical Processes: Photovoltaics and Charge Transfer in Nanomaterials, Mesilla, NM, January 2016.
- *"A few roadblocks on the way toward efficient perovskite photovoltaics"* (invited talk), PacificChem 2015, Honolulu, Hawaii, December 2015.
- *"A few lessons from non-adiabatic excited state dynamics simulations of large molecules"* (invited talk), PacificChem 2015, Honolulu, Hawaii, December 2015.
- *"A few roadblocks on the way toward efficient perovskite photovoltaics"* (invited seminar), Moscow State University (MSU), Moscow, Russia, November 2015.
- *"A journey to the land of excited state dynamics in organic semiconductors"* (invited colloquium), Skolkovo Institute of Science and Technology (SkolTech), Moscow, Russia, November 2015.
- *"First principle calculations of electronic transport in organic and bio-systems using atomistic structures"* (invited talk), Biological Electron Transfer Meeting, Research Triangle Park, NC, September 2015.
- *"A few roadblocks toward efficient perovskite photovoltaics"* (invited talk), Penn Conference in Theoretical Chemistry, University of Pennsylvania, Philadelphia, July 2015.
- *"Chemical functionalization and optical properties of carbon nanotube materials"* (invited talk), Telluride Workshop on Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, July 2015.
- *"A few roadblocks toward efficient perovskite photovoltaics"* (invited talk), Telluride Workshop on Spontaneous Coherence and Collective Dynamics, Telluride, CO, July 2015.
- *"Quantum chemistry, DFT and excited state molecular dynamics: modeling of functional electronic materials"* (invited lecture), 9th Q-bio Summer School,University of New Mexico, Albuquerque, July, 2015.
- *"Toward efficient perovskite photovoltaics"* (invited talk), 11th International Conference on Optical Probes, Hong Kong, HK, June 2015.
- *"Non-adiabatic excited state dynamics simulations of extended molecular systems"* (invited lecture), Kyoto University, Kyoto, Japan, June 2015.
- *"From engineering interfaces in soft electronic materials to efficient perovskite photovoltaics"*, (invited lecture), Kyoto University, Kyoto, Japan, June 2015.

- *"From engineering interfaces in soft electronic materials to efficient perovskite photovoltaics"* (invited seminar), University California, Santa Barbara, CA, May 2015.
- *"From engineering interfaces in soft electronic materials to efficient perovskite photovoltaics"*, (invited lecture), University of Southern California, Los Angeles, CA, May 2015.
- *"Multiscale DFT modeling of functional electronic materials"*, (invited lecture), University of Southern California, Los Angeles, CA, May 2015.
- *"Non-adiabatic excited state dynamics simulations of extended molecular systems"* (invited lecture), University of Southern California, Los Angeles, CA, May 2015.
- *"From engineering interfaces in soft electronic materials to efficient perovskite photovoltaics"* (invited colloquium), North Dakota State University, Fargo, ND, May 2015.
- *"From engineering interfaces in soft electronic materials to efficient perovskite photovoltaics"* (invited seminar), University of Rochester, Rochester, NY, March 2015.
- *"Evolution of photoexcited states in extended molecular chromophores"* (invited talk), 249th ACS National Meeting, Denver, CO, March 2015.
- *"Evolution of photoexcited states in extended molecular chromophores"* (invited talk), 55th Sanibel Symposium, St. Simons Island, Georgia, February 2015.
- *"Evolution of photoexcited states in extended molecular chromophores"* (invited colloquium), Department of Physics and Astronomy, the University of Utah, Salt Lake City, UT, February 2015.
- *"Theoretical insights into multiscale electronic processes in organic photovoltaics"* (invited talk), Materials Research Society (MRS) Fall Meeting, Boston, MA, December 2014.
- *"Photoexcited conjugated chromophores: conformational dynamics, relaxation pathways and energy transfer"* (invited talk), Materials Science and Engineering Conference, San Antonio, TX, October 2014.
- *"Photoexcited conjugated chromophores: conformational dynamics, relaxation pathways and energy transfer"* (invited seminar), Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, October 2014.
- *"Photoexcited conjugated chromophores: conformational dynamics, relaxation pathways and energy transfer"* (invited seminar), Department of Chemistry, University of South Dakota, Vermillion, SD, September 2014.
- *"Efficient Non-Adiabatic Excited State Dynamics Simulations in Extended Molecular Systems"* (invited talk), Telluride workshop: Excited States and Time-dependent Electronic Structure Theory, Telluride, CO, July 2014.
- *"Efficient Non-Adiabatic Excited State Dynamics Simulations in Extended Molecular Systems"* (invited talk), CUNY workshop: Theoretical and Practical Challenges in Nonadiabatic Quantum Dynamics, New York, NY, May 2014.
- *"Efficient Non-Adiabatic Excited State Dynamics Simulations in Extended Molecu¬lar Systems"* (invited colloquium), Department of Materials Science and Engineering, Boston University, Boston, May 2014.
- *"Photoexcited Conjugated Chromophores: Conformational Dynamics, Relaxation Pathways, and Energy Transfer"* (invited seminar), Department of Chemistry, Michigan State University, East Lansing, April 2014.

- *"Exciton Scattering approach for conjugated macromolecules: from electronic spectra to electron-phonon coupling"* (invited talk), Annual March Meeting of the APS, Denver, CO, March 2014.
- *"Life of photoexcited conjugated chromophores: the movie"* (invited talk), Materials Research Society (MRS) Fall Meeting, Boston, MA, December 2013.
- *"Life of photoexcited conjugated chromophores: the movie"* (invited talk), CECAM workshop: Quantum Dynamics in Molecular and Nano-Materials, Tel-Aviv, Israel, November 2013.
- *"Dynamics of excitons and phonons at the nanoscale"* (invited colloquium), Nanyang Technological University, Singapore, October 2013.
- *"Dynamics of excitons and phonons at the nanoscale"* (invited colloquium), Skolkovo Institute of Science and Technology (SkolTech), Moscow, Russia, October 2013.
- *"Life of photoexcited conjugated chromophores: the movie"* (invited talk), IPAM Workshop on Solar Cells, UCLA, Los Angeles, CA, September 2013.
- *"Localization of electronic excitations in organic semiconductors: theoretical views from different angles"* (invited talk), 246th ACS National Meeting, Indianapolis, IN, September, 2013.
- *"Localization of electronic excitations in organic semiconductors: theoretical views from different angles"* (invited talk), Telluride Workshop on Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, July 2013.
- *"Life of photoexcited conjugated chromophores: the movie"* (invited talk), 10th International Conference on Optical Probes, Durham, UK, July 2013.
- *"Localization of electronic excitations in organic semiconductors: theoretical views from different angles"* (invited seminar), Cambridge University, Cambridge, UK, July 2013.
- *"Localization of electronic excitations in organic semiconductors: theoretical views from different angles"* (invited seminar), Imperial College, London, UK, July 2013.
- *"Localization of Electronic Excitations in Carbon Nanotubes and Cycloparaphenylenes"* (invited talk), 5th International Conference on Nanotube Optics and Nanospectroscopy (WONTON 2013), Santa Fe, NM, June, 2013
- *"Localization of electronic excitations in organic semiconductors: theoretical views from different angles"* (invited colloquium), University of Central Florida, Orlando, FL, April 2013.
- *"Localization of electronic excitations in organic semiconductors: theoretical views from different angles"* (invited colloquium), University of Rochester, Rochester, NY, April 2013.
- *"Modeling of Energy and Charge Transfer in Organic Conjugated Materials"* (invited talk), 22nd Winter Inter-American Photochemical Society Meeting, Sarasota, Florida, January, 2013
- *"Modeling of Energy Transfer and Conformational Dynamics in Organic Conjugated Materials"* (invited seminar), Kyoto University, Kyoto, Japan, December 2012.
- *"Theoretical Modeling of Energy Transfer Mechanisms in Artificial Light-Harvesting Complexes"* (invited talk), International Workshop on Coherent Energy Transport and Optimization in Photosynthesis, Nanyang Technological University (NTU), Singapore, December 2012.

- *"Modeling of Energy and Charge Transfer in Organic Conjugated Materials"* (invited talk), International Workshop on Computational Methods for Complex Systems, Hong Kong University (HKU), Hong Kong, December, 2012.
- *"Modeling of Energy Transfer and Conformational Dynamics in Organic Conjugated Materials"* (invited talk), Workshop on Bio-Nano Interfaces and Architectures for Energy Conversion Santa Fe NM, November 2012.
- *"Modeling of Energy and Charge Transfer in Organic Conjugated Materials"* (invited seminar), University of Houston, Houston TX, October 2012.
- *"Dynamics of excitons and phonons in conjugated polymers and carbon nanotubes"* (invited seminar), University of Oregon, Eugene OR, October 2012.
- *"Multiscale Modeling of Electronic Excitations and Energy Transfer in Organic Conjugated Materials"* (invited talk), The Molecular Foundry 2012 Annual User Conference, Berkeley, CA, October 2012.
- *"Modeling of light-harvesting at the nanoscale"* (invited talk), 9th LANSCE Neutron Scattering School, Los Alamos, NM, September, 2012
- *"Energy and charge transfer in conjugated polymers: Beyond the Forster and Marcus theories"* (invited talk), 244th ACS National Meeting, Philadelphia, PA, August 2012.
- *"Vibrational Modes in Non-Adiabatic Excited State Dynamics of Conjugated Molecules"* (invited talk), Conference on Nanomaterials: Theory and Computation, Telluride, CO, July 2012.
- *"Dynamics of excitons and phonons in conjugated polymers and semiconductor quantum dots"* (invited talk), 10th International Conference on Excitonic Processes in Condensed Matter, Nanostructured and Molecular Materials (EXCON2012), Groningen, the Netherlands, July, 2012.
- *"Photoluminescence and Chemical Defects in Carbone Nanotubes"* (invited seminar), University of Mons Hainaut, Mons, Belgium, June 2012.
- *"To hop or not to hop: Excited state dynamics and energy transfer in organic molecules"* (invited talk), 243th ACS National Meeting, San Diego, CA, March 2012.
- *"Modeling of excited state dynamics and energy transfer in organic molecules"* (invited talk), 52th Sanibel Symposium, St. Simons Island, Georgia, February 2012.
- *"Dynamics of excitons and phonons in conjugated polymers and quantum dots"* (invited seminar), Carnegie Mellon University, Pittsburgh, PA, January 2012.
- *"Dynamics of excitons and phonons in conjugated polymers and quantum dots"* (invited seminar), University of Arizona, Tuscon, AZ, January 2012.
- *"Dynamics of excitons and phonons at the nanoscale"* (invited seminar), University of Wyoming, Laramie, WY, October 2011.
- *"From excitons and phonons to dynamics and transport in nanoscale materials"* (invited talk), 242th ACS National Meeting, Denver, CO, August 2011.
- *"Modeling of photoinduced relaxation pathways in conjugated polymers"* (invited talk), 242th ACS National Meeting, Denver, CO, August 2011.
- *"Conjugated organics: pushing TDDFT limits and lessons learned"* (invited talk), 2011 Gordon Research Conference on Time-dependent Density Functional Theory, Biddeford, ME, August 2011.

- *"Modeling of photoinduced relaxation pathways in conjugated polymers and carbon nanotubes"* (invited seminar), Cambridge University, Cambridge, UK, August 2011.
- *"Modeling of photoinduced relaxation pathways in conjugated polymers and carbon nanotubes"* (invited seminar), Imperial College, London, UK, August 2011.
- *"Dynamics of excitons and phonons at the nanoscale"* (invited seminar), Institute Politecnico di Milano, Milan, Italy, August 2011.
- *"Excitons and phonons at the nanoscale"* (invited seminar), University of Girona, Girona, Spain, August 2011.
- *"Modeling of photoinduced relaxation pathways in conjugated polymers"* (invited talk), Conference on Excited states and non-adiabatic processes in complex systems, Girona, Spain, August 2011.
- *"Modeling of photoinduced relaxation pathways in conjugated polymers"* (invited talk), American Conference on Theoretical Chemistry, Telluride, CO, July 2011.
- *"Modeling of photoinduced relaxation pathways in conjugated polymers"* (invited talk), Telluride Workshop on Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, July 2011.
- *"Excitons and phonons in carbon nanotubes"* (invited talk), Telluride Workshop on Spontaneous Coherence and Collective Dynamics, Telluride, CO, July 2011.
- *"Optical Control of Conjugated Oligomer Planarity"* (invited talk), Annual March Meeting of the APS, Dallas, TX, March 2011.
- *"Multiscale modeling of excited states and non-adiabatic dynamics in organic conjugated materials"* (invited seminar), Department of Chemistry, University of California, San Diego, CA, January 2011.
- *"Excitons and phonons in disordered nanoscale materials"* (invited talk), PacificChem 2010, Honolulu, Hawaii, December 2010.
- *"Modeling of nonadiabatic photoinduced dynamics and energy transfer in conjugated molecules"* (invited talk), PacificChem 2010, Honolulu, Hawaii, December 2010.
- *"Modeling of Non-adiabatic Photoinduced Dynamics and Energy Transfer in Conjugated Polymers"* (invited seminar), Department of Chemistry, Temple University, Philadelphia, PA, December 2010.
- *"Multiscale modeling of excited states and non-adiabatic dynamics in organic conjugated materials"* (plenary talk), Conference on Current Trends in Computational Chemistry (CCTCC-19), Jackson, MS, October, 2010.
- *"Modeling of Non-adiabatic Photoinduced Dynamics for Photovoltaic Applications"* (invited talk), Workshop on Theory and Simulation of Nano Scale Materials, CINT, Albuquerque, NM, October 2010.
- *"Modeling of Non-adiabatic Photoinduced Dynamics and Energy Transfer in Conjugated Molecules"* (invited talk), XXII International Conference on Raman Spectroscopy (ICORS-2010), Boston, MA, August, 2010.
- *"Modeling of Non-adiabatic Photoinduced Dynamics and Energy Transfer in Conjugated Molecules"* (invited talk), SPIE meeting on Optics and Photonics, San Diego, CA, August 2010.

- *"Modeling of Non-adiabatic Photoinduced Dynamics and Energy Transfer in Conjugated Molecules"* (invited talk), ICCE-18 (International Conference on Composites/Nano Engineering), Anchorage, AL, July, 2010
- *"Modeling of Non-adiabatic Photoinduced Dynamics and Energy Transfer in Conjugated Molecules"* (invited talk), CECAM workshop on Quantum transport and dynamics in materials and biosystems: From molecular mechanisms to mesoscopic functionality, Dublin, Ireland, May 12, 2010
- *"Modeling of Electronic Structure and Photoinduced Dynamics in Electronic materials"* (invited seminar), Photovoltaics workshop, University of New Mexico, Albuquerque, NM, April 2010.
- *"Excited State Dynamics and Energy Transfer in Quantum Dots"* (invited seminar), Cell Biology and Neuroscience Center for High Technology Materials, University of New Mexico, Albuquerque, NM, March 2010.
- *"Dynamics of excitons and phonons in disordered organic and inorganic materials"*, (invited seminar), Department of Chemistry, Purdue University, Lafayette, IN, February 2010.
- *"Multiscale modeling of excited states and spectroscopy at the nanoscale"* (invited seminar), Department of Chemistry, Purdue University, Lafayette, IN, February 2010.
- *"Modeling of Photoinduced Dynamics at the Nanoscale"* (invited seminar), Department of Chemistry, University of New Mexico, Albuquerque, NM, January 2010.
- *"Excitons and phonons in disordered nanoscale materials"* (invited seminar), Department of Chemistry, University of Florida, FL, January 2010.
- *"Modeling of Photoinduced Dynamics at the Nanoscale"* (invited colloquium), Condensed Matter Science Colloquium, Los Alamos National Laboratory, Los Alamos, NM, January 2010.
- *"Dynamics of excitons and phonons in disordered nanoscale materials"* (invited seminar), Center for Excitonics, Massachusetts Institute of Technology (MIT), Cambridge, MA, December 2009.
- *"Modeling of Photoinduced Dynamics at the Nanoscale"* (invited seminar), Department of Chemistry, University of Rochester, Rochester, NY, November 2009.
- *"Modeling of Photoinduced Dynamics at the Nanoscale"* (keynote lecture), Southwest Theoretical Chemistry Conference, Houston, TX, October 2009
- *"Conjugated polymers for light harvesting applications: Theoretical insights"* (invited talk), ICCE-17 (International Conference on Composites/Nano Engineering), Honolulu, HI, August 2009.
- *"Non-adiabatic excited state dynamics in ligated quantum dots and conjugated molecules"* (invited talk), Telluride Workshop on Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, July 2009.
- *"Electronic properties of amorphous conjugated polymers and organic/semiconductor interfaces"* (invited talk), the 8th International Conference on Optical Probes of Conjugated Polymers and Organic Nanostructures (OP 2009), Beijing, June 2009.
- *"Multiscale modeling of electronic excitations at the nanoscale"* (invited seminar), Hong Kong University of Science and Technology, Hong Kong, June 2009.
- *"Functionalized quantum dots and conjugated polymers for light harvesting applications: Theoretical insights"* (invited seminar), Hong Kong University, Hong Kong, June 2009.

- *"Functionalized quantum dots and conjugated polymers for light harvesting applications: Theoretical insights"* (invited seminar), Kyoto University, Kyoto, Japan, May 2009.
- *"Functionalized quantum dots and conjugated polymers for light harvesting applications: Theoretical insights"* (invited talk), 237th ACS National Meeting, Salt Lake City, UT, March 2009.
- *"Multiscale modeling of electronic excitations at the nanoscale"* (invited talk), 237th ACS National Meeting, Salt Lake City, UT, March 2009.
- *"Photoinduced dynamics in functionalized quantum dots and other nanostructures"* (invited talk), Workshop on Wave Function Engineering and Coherent Control in Nanostructured Materials, LANL, Los Alamos, NM, February 2009.
- *"Functionalized quantum dots and conjugated polymers for light harvesting applications: Theoretical insights"* (invited seminar), Department of Chemistry, University of California, Riverside, CA, February 2009.
- *"Multiscale Modeling of Electronic Excitations at the Nanoscale"* (invited seminar), University de Rennes, Rennes, France, December 2008.
- *"Functionalized quantum dots and conjugated polymers for light harvesting applications: Theoretical insights"* (invited talk), Helsinki University of Technology/University of Helsinki conference Towards Reality in Nanoscale Materials '08, Levi, Finland, December, 2008.
- *"Functionalized quantum dots for light harvesting applications: Theoretical insights"* (invited seminar), University of Mons Hainaut, Mons, Belgium, December 2008.
- *"Functionalized quantum dots and conjugated polymers for light harvesting applications: Theoretical insights"* (invited seminar), Department of Physics, Michigan State University, East Lansing, MI, November 2008.
- *"Functionalized quantum dots and conjugated polymers for light harvesting applications: Theoretical insights"* (invited talk), IMA conference on Scientific Challenges in Solar Energy Conversion and Storage, Minneapolis, MN, November 2008.
- *"Photoinduced dynamics in carbon nanotubes and colloidal quantum dots"* (invited talk), 92nd OSA National Meeting, Rochester, NY, October 2008.
- *"Multiscale Modeling of Electronic Excitations at the Nanoscale"* (invited talk), Institute for Multiscale Materials Studies Workshop, Los Alamos, NM, September 2008.
- *"Electronic properties of amorphous conjugated polymers and organic/semiconductor interfaces"* (invited talk), SPIE meeting on Optics and Photonics, San Diego, CA, August 2008.
- *"Excitonic Effects in Low-Dimensional Nanoscale Materials"* (invited seminar in T-11 group), Los Alamos, NM, May 2008.
- *"Electronic properties of amorphous conjugated polymers and bio-molecular adsorbates"* (invited talk), 235th ACS National Meeting, New Orleans, LA, April 2008.
- *"First-principles calculations of photoinduced dynamics in carbon nanotubes"* (invited talk), Annual March Meeting of the APS, New Orleans, LA, March 2008.
- *"Electronic properties of conjugated polymers and DNA adsorbed on a surface"* (invited talk), 48th Sanibel Symposium, St. Simons Island, Georgia, February 2008.
- *"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"* (invited talk), 233th ACS National Meeting, Chicago, IL, March 2007.
- *"Excitons and spectroscopy of carbon nanotubes and pi-conjugated polymers"* (invited seminar), University of Mons Hainaut, Mons, Belgium, December 2006.
- *"Selected applications of quantum chemistry to functional optical materials"* (invited seminar), 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"* (invited seminar), University de Rennes, Rennes, France, December 2006.
- *"Selected applications of quantum chemistry to functional optical materials"* (invited seminar), 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 talk), 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 Nanocrys-tals: 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 and Astronomy, 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"*, (invited lecture), Winter School in Theoretical Chemistry on Nanophotonics, Department of Chemistry, University of Helsinki, Helsinki, Finland, December 2005.
- *"Adiabatic and nonadiabatic excited state dynamics in molecular aggregates"*, (invited lecture), Winter School in Theoretical Chemistry on Nanophotonics, Department of Chemistry, University of Helsinki, Helsinki, Finland, December 2005.
- *"Nonlinear optical response of organic electronic materials"*, (invited lecture), Winter School in Theoretical Chemistry on Nanophotonics, Department of Chemistry, University of Helsinki, Helsinki, Finland, December 2005.
- *"Electronic structure and vibrational interactions in colloidal quantum dots and their assemblies"* (invited lecture), 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"* (invited 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"* (invited 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"* (invited talk), 2001 MRS Fall National Meeting, Boston, MA, November 2001.
- *"Semiempirical methods for excited state dynamics of conjugated molecules"* (invited 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"* (invited 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 (over 300 articles and book chapters):

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

Google Scholar citations: https://scholar.google.com/citations?user=jHs7JoEAAAAJ&hl=en
ResearcherID profile: http://www.researcherid.com/rid/B-5556-2009
Scopus profile: https://www.scopus.com/authid/detail.uri?authorId=7003665075
ORCID profile: http://orcid.org/0000-0001-5547-3647

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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 (journal cover page) **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).
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11. S. Tretiak, V. Chernyak, and S. Mukamel, *"Real-space analysis of electronic excitations in free-base (H2P) 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).
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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).
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24. V. Chernyak, S. Tretiak, and S. Mukamel, *"Electronic versus vibrational optical non-linearities of push-pull polymers,"* Chem. Phys. Lett., **319**, 261 – 264 (2000).
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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. V. Chernyak, S. Tretiak, M. Schulz, E. V. Tsiper, and S. Mukamel, *"Krylov-space algorithms for time-dependent Hartree-Fock and density functional computations,"* J. Chem. Phys., **113**, 36 – 43 (2000).
29. 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).
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33. 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).
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44. 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).
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46. S. Tretiak and V. Chernyak, *"Resonant nonlinear polarizabilities in the time-dependent density functional (TDDFT) theory,"*J. Chem. Phys., **119**, 8809 – 8823 (2003).
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