Braden M. Weight

Theoretical Division (T-1), Mail Stop B221
Los Alamos National Laboratory
Los Alamos, NM 87544, U.S.A.
(701) 202 0603
Google Scholar
bweight@ur.rochester.edu
bradenmweight.github.io
github.com/bradenmweight

Education

2025 **Director's Postdoctoral Fellow**, *Los Alamos National Laboratory*, Los Alamos, NM.

2020–2025 **Doctor of Philosophy in Physics**, *University of Rochester*, Rochester, NY.

2020–2022 **Master of Science in Physics**, *University of Rochester*, Rochester, NY.

2018–2020 Master of Science in Physics, North Dakota State University, Fargo, ND.

2014–2018 Bachelor of Science in Physics,
Bachelor of Science in Chemistry,
North Dakota State University, Fargo, ND.

Research Interests

Light-Matter Interactions

Polaritonic chemistry has become the leading direction to control a multitude of processes, such as charge transfer, selective bond breaking, and excited state dynamics. An exciton-polariton is an entangled state of light and matter in which the native electronic and photonic quantum states hybridize to form new states. These new states can be tuned in various ways to modify and produce unique chemical and physical properties such as potential energy landscapes or the electronic density distributions of molecules and materials.

Quantum Dynamics The versatility and increasing general interest of nanotechnology is without bound and is of great importance to the world. Studying the time-dependence of these many-body systems is challenging and requires the development of new and efficient methods that give accuracy between the expensive wavepacket methods (AIMS, MCTDH, MC-Ehrenfest, etc.) and the mixed quantum-classical Ehrenfest method.

Structure

Electronic properties of materials is a vast and ever-growing realm of research. My ambitions in this field are far-reaching from molecules to materials. Depending on the chemical system, I employ a wide range of approaches such as quantum Monte Carlo, coupled cluster, density functional, and semi-empirical/tight-binding theories.

Collaboration

One cannot do great science alone. I strive to foster collaboration within all aspects of my career, both between theorists (WIRES 2025, PRA 2024, PRA 2024, Chem. Rev. 2023, PCCP Pers. 2023, JCP 2022) as well as between theory and experiment (in review at Nat. Commun. Mater., JACS 2025, Nat. Commun. 2022, JPCL 2023, ACS Nano 2021, ACS Nano 2021), evidenced by these collaborative works

Honors and Awards

2025 Outstanding Dissertation Award in the College of Natural Science (Mathematics, Biology, Chemistry, Physics, and Astronomy), *University of Rochester*, Rochester, NY
\$1,000 Award – One award per year

2025 Director's Postdoctoral Fellowship, *Los Alamos National Laboratory*, Los Alamos, NM **\$10,000 Award**

2025 1st-place Award at Graduate Research Day, *University of Rochester*, Rochester, NY \$300 Award

2023 Zerner Graduate Student Award, 62nd Sanibel Symposium: Quantum Theory Project, St. Augustine Beach, FL \$500 Award

2018 1st Place Award at the 58th Annual Sanibel Symposium: Quantum Theory Project in the undergraduate poster competition, St. Simons Island, GA **\$100 Award**

2017 4th place in NDSU EXPLORE for the poster competition, Fargo, ND

2017 North Dakota State University Physics Achievement Award, Fargo, ND \$100 Award

2016 1st place award in Solving Real World Problems: Graduate Research Exposition - Interdisciplinary Celebration of Research for best undergraduate presentation, Fargo, ND
\$100 Award

2015–2018 James Sigihara Scholarship for academic excellence, North Dakota State University, Fargo, ND \$100 Award / Semester

Research Experience

2025-Present Director's Postdoctoral Fellow, Dr. Y. Zhang / Dr. S. Tretiak, Los Alamos National Laboratory.

Quantum Dynamics and Magnetic Interactions in Ab Initio Molecular Cavity Quantum Electrodynamics,

- o Developing simulation tools for the quantum dynamics of large ab initio systems within a quantum electrodynamic (QED) framework
- Exploring chiroptical effects in molecules and materials inside and outside quantized cavity fields
- Inducing spin-phase transitions in heavy-element metal-organic complexes to elucidate novel properties Publications: In Preparation 2025, arXiv 2025, ACS Nano 2025

Proposal Development: Tier 2 Institutional Computing (IC, LANL) Proposal as lead PI

Software Development: OpenMS, Polariton NAMD

Graduate Research Assistant, Dr. P. Huo, University of Rochester. 2020-2025

Cavity Quantum Electrodynamics for Molecular and Material Simulation,

 Developed computational methods and tools to examine the ground and excited states of hybrid electron-photon-nuclear systems using time-dependent density functional theory (TD-DFT) Publications: WIRES Comp. Mol. Sci. 2025, PRA 2025, JPCA 2025 JACS 2024; PRA 2024; PRB

2024; JPCL 2023; Chem. Rev. 2023

Software Development: Ab Initio Polaritons

Graduate Research Assistant, Dr. Y. Zhang / Dr. S. Tretiak, Los Alamos National Laboratory. 2022-2025

Summer GRA Ab initio Cavity Quantum Electrodynamics for Molecular and Material Simulation,

o Formulated novel quantum chemistry approaches (QED-Hartree-Fock, QED-coupled cluster, QEDquantum Monte Carlo) toward the simulation of ab initio polaritonic properties

Publications: arXiv 2025, PRA 2024; PCCP Perspective 2023

Software Development: OpenMS

2020-2025 Graduate Research Assistant, Dr. P. Huo, University of Rochester.

Ab initio Nonadiabatic Simulations of Photochemistry,

• Implemented/benchmarked various state-of-the-art mixed quantum-classical dynamics approaches, e.g., linearized and partially linearized spin-mapping (spin-LSC, spin-PLDM), symmetric quasi-classical (SQC) Publications: JCP 2021; JCP 2022; JCP 2025

Software Development: SQD, SHARC-SQC, SHARC-spinLSC, SHARC-spinPLDM

2018-2025

Undergraduate/Graduate Research Assistant, Dr. S. Tretiak / Dr. B. Gifford / Dr. S. Kilina,

Summer GRA Los Alamos National Laboratory / North Dakota State University.

Ab initio Simulations of Low-dimensional Nanomaterials,

o Collaborated with experimental colleagues (Dr. Steve Doorn, Dr. Han Htoon, Dr. Ming Zheng) in calculations of nuclear and electronic spectroscopies of carbon nanotubes

Publications: RSC Appl. Interfaces 2024, JPCL 2023; ACS Nano 2023; Nat. Commun. 2022; JPCL 2022; JPCL 2021; JPCC 2021; ACS Nano 2020; Nano Lett. 2019; JPCC 2019

Teaching Experience

2022-Present Course Development - Introduction to Computational Quantum Mechanics, Rochester, NY.

- Composed high-level course curriculum, including syllabus, lecture notes/codes, homeworks/solutions.
- Covered topics include: Python programming, Numerical Calculus, and Quantum/Classical Dynamics
- o Freely available course materials with notes and many example Python codes: Course Website

2018-Present Research Mentor, North Dakota State University / University of Rochester Los Alamos National Laboratory. One-on-one Instruction

- Mentored 5+ undergraduate/graduate students
- Fostered critical thinking, data presentation, and writing skills
- o Recent first-author articles of mentees: ACS Nano 2025, JPCA 2025

2020–2021 **Teaching Assistant – Physics**, *University of Rochester*, Rochester, NY.

Full-Class Instruction

o Facilitated undergraduate physics-based laboratories

2018–2020 Teaching Assistant – Physics, North Dakota State University, Fargo, ND.

Full-Class Instruction

Facilitated undergraduate physics-based laboratories

2018–2020 High School Substitute Teacher, Fargo Public Schools, Fargo, ND.

Full-Class Instruction

- Certified K-12 license granted by the Education Standards and Practices Board of North Dakota
- Communicated materials with audiences of varying ages (K-12)
- 2015–2016 Personal Tutor, Self-Employed, Fargo, ND.

One-on-one Tutoring by Appointment,

Tutored honors chemistry and physics

2015 Academic Tutor, ACE Tutoring Center, North Dakota State University, Fargo, ND.

Group Academic Tutoring,

• Facilitated simultaneous tutoring of large groups (5-20) on a variety of subjects (mathematics, chemistry, physics, English)

Skills and Software Familiarity

Algorithms: Velocity-Verlet, Runge-Kutta; Davidson, split operator, Chebyshev, Crank-Nicholson; self-consistent field (e.g., Hartree-Fock), numerical optimization (e.g., Newton-Raphson)

Proposal Contributed to various open-science proposals – NSF CHE-2124398, NSF CHE-2244683, NSF OAC-2311442,

Development: AFOSR FA9550-23-1-0438

Languages: Python, Linux, LaTeX, Mathematica, FORTRAN77/95, JAVA, C, C++

Packages: Gaussian, SHARC, VASP, MultiWFN, Q-CHEM, LAMMPS, TINKER, VMD, VESTA, DFTB+, CP2K, Grimme-xTB

Plotting: Origin, Excel, Python/Matplotlib, MATLAB, GNUPLOT

Computing: High-performance computing (local and national, e.g., NERSC), OpenMP/MPI Parallelization

Reviewing Responsibilities

ACS Nano – American Chemical Society
ACS In Focus – American Chemical Society
J. Phys. Chem. – American Chemical Society
J. Appl. Phys. – American Institute of Physics

Volunteer Work

2019–2020 Vice President (and Acting President) of Graduate Physics Association, Performed administrative duties commensurate to running a graduate organization, which supports physics students to attend conferences and promotes various outreach activities, North Dakota State University, Fargo, ND.
60 Hours

2019 North Dakota Science Olympiad Event Official, Coordinated and administered the "Sounds of Music" event, which included writing and grading tests as well as adjudicating home-made instruments, Fargo, ND.
20 Hours

2016–2022 **Physics Outreach Events**, Physics demos for various activities including elementary schools, community fairs, and other various events , Fargo, ND.

30 Hours

Publications – h-index: 15/13, Total Citations: 661/430, (Google Scholar / Web Of Science)

- Oct. 2025 **31**. **Braden M. Weight***, Sergei Tretiak, and Yu Zhang* Cavity-induced Modifications to Circular Dichorism Spectroscopy. Los Alamos National Laboratory, Los Alamos, NM. *in preparation*, 2025
- Oct. 2025 **30**. **Braden M. Weight***, Aaron Forde, Victor Freixas, Sergei Tretiak* A Visual Understanding of Circular Dichroism Spectroscopy: Computational Insights. Los Alamos National Laboratory, Los Alamos, NM. *in preparation*, 2025
- Sep. 2025 **29**. **Braden M. Weight***, Aaron S. Rury, Yihan Shao, Todd D. Krauss, and Pengfei Huo.* Ab Initio Simulations of Polariton Spectra of ZnTPP Collectively Coupled Inside an Optical Cavity. Los Alamos National Laboratory, Los Alamos, NM.

 in preparation, 2025
- Aug. 2025 **28**. Yih-Ren Chang, Jacob Fortner, Vigneshwaran Chandrasekaran, Brendan J. Gifford, **Braden M. Weight**, Stephen K. Doorn, Han Htoon,* Yuichiro K. Kato,* Sergei Tretiak*, YuHuang Wang.* Quantum Defects in Carbon Nanotubes as Single-Photon Sources. Los Alamos National Laboratory, Los Alamos, NM. *Submitted to Nat. Commun. Mat.*, 2025

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^{*} Corresponding author

- Aug. 2025 27. Dinesh Thapa,* Yulun Han, Braden M. Weight, Grace Tiffany, Dmitri Kilin, Sergei Tretiak, and Svetlana Kilina.* Singlet and triplet excitations in chemically functionalized single-walled carbon nanotubes. Los Alamos National Laboratory, Los Alamos, NM.
 Submitted to J. of Mat. Chem. C, 2025
- May 2025 **26. Braden M. Weight** and Yu Zhang.* Auxiliary Field Quantum Monte Carlo for Electron-Photon Correlation. Los Alamos National Laboratory, Los Alamos, NM. *arXiv*, 2025, DOI: 10.48550/arXiv.2505.16021 **Citations: 3/0**

- Aug. 2025 25. Grace Tiffany, Amara Arshad, Braden M. Weight, August Amb, Aaron Forde, Brendan J. Gifford, Alexander Star, Sergei Tretiak,* Dmitri Kilin,* Svetlana Kilina.* Inducing Circular Dichroism in Carbon Nanotubes by Chemical Defects. Los Alamos National Laboratory, Los Alamos, NM.
 IF: 15.8 ACS Nano 2025, 19, 33, 30476–30486
 Citations: 0/0
- July 2025 **24**. **Braden M. Weight*** and Pengfei Huo.* Ab Initio Approaches to Simulate Molecular Polaritons and Quantum Dynamics. University of Rochester, Rochester, NY. **IF: 11.4** *Wiley Interdisciplinary Reviews: Comp. Mol. Sci.* 15, no. 4 (2025): e70039 **Citations: 5/2**
- July 2025 **23**. **Braden M. Weight*** and Pengfei Huo.* Stochastic-Chebyshev-expansion approach for the simulation of linear polariton spectroscopy in the collective-coupling regime. University of Rochester, Rochester, NY. **IF: 3.0** *Phys. Rev. A* 112, 013713 (2025) **Citations: 0/0**
- June 2025 **22.** Jialong Wang, **Braden M. Weight**,* and Pengfei Huo.* Quantum Investigating Cavity Quantum Electrodynamics-Enabled Endo/Exo- Selectivities in Diels-Alder Reactions. University of Rochester, Rochester, NY. **IF: 2.7** *J. Phys. Chem. A* 2025, 129, 25, 5458–5468 **Citations: 3/1**
- Feb. 2025 **21. Braden M. Weight*** and Pengfei Huo.* *Ab initio* on-the-fly simulations of photochemistry using spin-mapping non-adiabatic dynamics. University of Rochester, Rochester, NY. **IF: 4.4** *Journal of Chemical Physics* 162, 084105 (2025) **Citations: 3/3**
- May 2024 **20**. **Braden M. Weight**,* Daniel J. Weix,* Zachary Tonzetich, Todd D. Krauss, and Pengfei Huo.* Cavity Quantum Electrodynamics Enables para- and ortho- Bromination of Nitrobenzene. University of Rochester, Rochester, NY. **IF: 14.4** *Journal of the American Chemical Society*, 2024, 146, 23, 16184–16193 **Citations: 22/16**
- Mar. 2024 19. Michael A.D. Taylor,* Braden M. Weight,* and Pengfei Huo.* Reciprocal Asymptotically Decoupled Hamiltonian for Cavity Quantum Electrodynamics. University of Rochester, Rochester, NY.
 IF: 3.9 Physical Review B, 109, 104305 (2024)

 Citations: 9/3
- Mar. 2024 **18**. **Braden M. Weight***, Sergei Tretiak, and Yu Zhang.* A Diffusion Quantum Monte Carlo Approach to the Polaritonic Ground State. Los Alamos National Laboratory, Los Alamos, NM. **IF: 3.0** *Physical Review A*, 109, 032804 (2024) **Citations: 31/14**
- Nov. 2023 17. Braden M. Weight, Brendan J. Gifford*, Grace Tiffany, Elva Henderson, Deyan Mihaylov, Dmitri Kilin, and Svetlana Kilina.* Optically Active Defects in Carbon Nanotubes via Chlorination: Computational Insights. University of Rochester, Rochester, NY.

 IF: 8.3 RSC Applied Interfaces, 2024, 1, 281–300

 Citations: 3/3
- Sept. 2023 16. Braden M. Weight, Xinyang Li, and Yu Zhang.* Theory and Modeling of Light-matter Interactions in Chemistry: Current and Future. Los Alamos National Laboratory, Los Alamos, NM. Invited by *Physical Chemistry Chemical Physics* to contribute a perspective article on light-matter interactions in chemistry.

 IF: 2.9 Physical Chemistry Chemical Physics, 2023, 25, 31554-31577

 Citations: 44/25
- July 2023 **15**. Arkajit Mandal,*† Michael A.D. Taylor,† **Braden M. Weight**,† Eric R. Koessler,† Xinyang Li, and Pengfei **Supp. Cover** Huo.* Theoretical Advances in Polariton Chemistry and Molecular Cavity Quantum Electrodynamics. University of Rochester, Rochester, NY. **Invited by Chemical Reviews** as part of a special issue on polariton chemistry **IF: 51.4** Chemical Reviews 2023, 123, 16, 9786–9879 **Citations: 240/151**
 - June 2023 14. Braden M. Weight,* Todd D. Krauss, and Pengfei Huo.* Investigating Molecular Exciton Polaritons Using Ab Initio Cavity Quantum Electrodynamics. University of Rochester, Rochester, NY.
 IF: 5.7 Journal of Physical Chemistry Letters 2023, 14, 25, 5901–5913
 Citations: 35/25
 - Mar. 2023 13. Braden M. Weight*, Andrew Sifain, Brendan J. Gifford, Han Htoon, and Sergei Tretiak.* On-the-fly Non-adiabatic Dynamics Simulations of Single-Walled Carbon Nanotubes with Covalent Defects. Los Alamos National Laboratory, Los Alamos, NM.
 IF: 15.8 ACS Nano 2023, 17, 7, 6208–6219
 Citations: 12/8
 - Jan. 2023 **12**. **Braden M. Weight**, Ming Zheng, and Sergei Tretiak.* Signatures of Chemical Dopants in Simulated Resonance Raman Spectroscopy of Carbon Nanotubes. Los Alamos National Laboratory, Los Alamos, NM. **IF: 5.7** *Journal of Physical Chemistry Letters*, 2023, 14, 5, 1182–1191 **Citations: 20/16**
 - Nov. 2022 11. Deping Hu,* Arkajit Mandal, Braden M. Weight, Pengfei Huo.* Quasi-Diabatic Propagation Scheme for Simulating Polariton Chemistry. University of Rochester, Rochester, NY.
 IF: 4.4 Journal of Chemical Physics, 157, 194109 (2022)

 Citations: 26/18

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[†] Authors contributed equally

- Aug. 2022 10. Yu Zheng, Yulun Han, Braden M. Weight, Zhiwei Lin, Brendan J. Gifford, Ming Zheng, Dmitri Kilin, Svetlana Kilina, Stephen K. Doorn, Han Htoon, and Sergei Tretiak. Photochemical spin-state control of binding configuration for tailoring organic color center emission in carbon nanotubes. Los Alamos National Laboratory, NM.
 - **IF: 14.7** *Nature Communications* 13, 4439 (2022) **Citations: 18/15**
- June 2022 9. Shahriar N. Khan, Braden M. Weight, Brendan J. Gifford, Sergei Tretiak,* and Alan Bishop.* Impact of Graphene Quantum Dot Edge Morphologies on Their Optical Properties. Los Alamos National Laboratory, NM.
 IF: 5.7 Journal of Physical Chemistry Letters 2022, 13, 25, 5801–5807
 Citations: 10/11
- Aug. 2021 **8. Braden M. Weight**, Arkajit Mandal, and Pengfei Huo.* *Ab initio* symmetric quasi-classical approach to investigate molecular Tully models. University of Rochester, Rochester, NY. **IF: 4.4** *Journal of Chemical Physics* 155, 084106 (2021) **Citations: 26/21**
- Aug. 2021 **7. Braden M. Weight**, Andrew E. Sifain, Brendan J. Gifford, Dmitri Kilin, Svetlana Kilina, and Sergei Tretiak.* Coupling between Emissive Defects on Carbon Nanotubes: Modeling Insights. Los Alamos National Laboratory,
- Feb. 2021 **6. Braden M. Weight**, Brendan J. Gifford, Sergei Tretiak, and Svetlana Kilina.* Interplay between Electrostatic Properties of Molecular Adducts and Their Positions at Carbon Nanotubes. Los Alamos National Laboratory, NM. **IF: 3.7** *Journal of Physical Chemistry C* 2021, 125, 8, 4785–4793 **Citations: 19/13**
- Jan. 2021 5. Yu Zheng,* Braden M. Weight, Andrew C. Jones, Vigneshwaran Chandrasekaran, Brendan J. Gifford, Sergei Tretiak, Stephen K. Doorn, Han Htoon.* Photoluminescence Dynamics Defined by Exciton Trapping Potential of Coupled Defect-States in DNA-Functionalized Carbon Nanotubes. Los Alamos National Laboratory, NM.
 IF: 15.8 ACS Nano 2021, 15, 1, 923–933
 Citations: 25/18
- Feb. 2020 **4.** Younghee Kim, Serguie V. Goupalov, **Braden M. Weight**, Brendan J. Gifford, Xiaowei He, Avishek Saha, Mijin Kim, Geyou Ao, YuHuang Wang, Ming Zheng, Sergei Tretiak, Stephen K. Doorn,* Han Htoon.* Hidden Fine Structure of Quantum Defects Revealed by Single Carbon Nanotube Magneto-Photoluminescence. Los Alamos National Laboratory, NM.
 - **IF: 15.8** ACS Nano 2020, 14, 3, 3451–3460 **Citations: 18/15**

Citations: 32/25

Citations: 7/5

Citations: 17/14

- Nov. 2019 **3**. Brendan J. Gifford, Avishek Saha, **Braden M. Weight**, Xiaowei He, Geyou Ao, Ming Zheng, Han Htoon, Svetlana Kilina, Stephen K. Doorn,* and Sergei Tretiak.* Mod(n-m,3) Dependence of Defect-State Emission Bands in Aryl Functionalized Carbon Nanotubes. Dept. of Physics, North Dakota State University. Los Alamos National Laboratory. NM.
 - **IF**: **10.8** *Nano Letters* 2019, 19, 12, 8503-8509
- Aug. 2019 **2**. Brendan J. Gifford, **Braden M. Weight**, and Svetlana Kilina.* Interplay between Conjugated Backbone Units and Side Alkyl Groups in Chirality Sensitive Interactions of Single Walled Carbon Nanotubes with Polyfluorenes, Dept. of Physics, North Dakota State University.
 - **IF**: **3.7** *Journal of Physical Chemistry C* **123** (40), 2019, 24807-24817
- Mar. 2018 1. Braden M. Weight and Alan R. Denton,* Structure and Stability of Charged Colloid-Nanoparticle Mixtures. Dept. of Physics, North Dakota State University.
 - IF: 4.4 Journal of Chemical Physics 148 (11), 2018, 114904

Presentations

- Sept. 4, 2025 **40**. Nonadiabatic Dynamics and the Chemical and Photophysical Properties of Molecular Exciton Polaritons, **Talk** Postdoctoral Seminar Series, Los Alamos National Laboratory, Los Alamos, NM.
- Aug. 21, 2025 **39**. Nonadiabatic Dynamics and the Chemical and Photophysical Properties of Molecular Exciton Polaritons, **Invited Talk** Telluride Science Workshop, Telluride, CO.
- June 19, 2025 38. Chemical and Photophysical Properties of Molecular Exciton Polaritons, Excited State Processes 2025, Santa Invited Talk Fe, NM.
- June 16, 2025 37., Cavity Quantum Electrodynamics Enables para- and ortho-Selective Electrophilic Bromination of Nitrobenzene, Poster, Excited State Processes 2025, Santa Fe, NM.
- Mar. 28, 2025 **36**., Cavity Quantum Electrodynamics Enables *para* and *ortho*-Selective Electrophilic Bromination of Nitrobenzene, Graduate Research Day, Poster, University of Rochester, NY.
- Feb. 27, 2025 **35**., Cavity Quantum Electrodynamics Enables *para-* and *ortho-*Selective Electrophilic Bromination of Nitrobenzene, **Talk** 64th Annual Sanibel Symposium St. Augustine Beach, FL.
- June 18, 2024 **34**., Cavity Quantum Electrodynamics Enables *para-* and *ortho-*Selective Electrophilic Bromination of Nitrobenzene, American Conference on Theoretical Chemistry (ACTC), Poster, University of North Carolina at Chapel Hill, NC.
- Mar. 6, 2024 33., A Diffusion Quantum Monte Carlo Approach to the Polaritonic Ground State, APS March Meeting Las Vegas, Talk NV.
- Feb. 27, 2024 **32**., Electrodynamics in the Chebyshev Basis for a Macroscopic Number of Molecules, 63th Annual Sanibel Symposium, Poster, St. Augustine Beach, FL.

- Aug. 18, 2023 31., A Diffusion Quantum Monte Carlo Approach to the Polaritonic Ground State, LANL Lightning Talk Los Talk Alamos, NM.
- Mar. 23, 2023 **30**., Investigating Molecular Exciton-Polaritons using Many-body Electronic Structure Theory with Cavity Quantum Electrodynamics, APS March Meeting Las Vegas, NV.
- Feb. 14, 2023 **29**., Investigating Molecular Exciton-Polaritons using Many-body Electronic Structure Theory with Cavity Quantum Electrodynamics, 62th Annual Sanibel Symposium, Poster, St. Augustine Beach, FL.
- Oct. 13, 2022 **28**., Properties of Molecular Exciton-Polaritons from Simple *ab Initio* Cavity Quantum Electrodynamics Calculations, Invited Talk NDSU Department of Chemistry Seminar, Fargo, ND.
- Oct. 5, 2022 27., Interfacial Charge Transfer in Rhodamine-based Dye-sensitized TiO2 Quantum Dots with *Ab Initio* Non-Talk adiabatic Excited State Dynamics Simulations, ACS North Eastern Regional Meeting (NERM) Rochester, NY.
- Oct. 4, 2022 **26**., Properties of Molecular Exciton-Polaritons from Simple *ab Initio* Cavity Quantum Electrodynamics Calculations, **Talk** ACS North Eastern Regional Meeting (NERM) Rochester, NY.
- June 2, 2022 **25**., Properties of Molecular Exciton-Polaritons: Coupling *Ab Initio* Calculations with Quantum Optics, ACS Middle Atlantic Regional Meeting (MARM), Poster, Trenton, NJ.
- Mar. 23, 2022 **24**., Properties of Molecular Exciton-Polaritons: Coupling *Ab Initio* Calculations with Quantum Optics, Graduate Research Symposium, Poster, Rochester, NY.
- Mar. 14, 2022 23., On-the-fly Exploration of Recent Spin-mapping Non-adiabatic Frameworks, Invited Speaker Department of Chemistry Poster Session, Poster, Rochester, NY.
- Oct. 21, 2021 **22**., Non-adiabatic Dynamics Simulations of Single-Walled Carbon Nanotubes with Topological sp3-defects: An On-the-fly NEXMD Study, Fall 2021 Bi-Annual Industrial Associates Symposium, Poster, Rochester, NY.
- Sep. 30, 2021 **21**., Non-adiabatic Dynamics Simulations of Single-Walled Carbon Nanotubes with Topological sp³-defects: An **Invited Talk** On-the-fly NEXMD Study, Virtual International Seminar on Theoretical Advancements (VISTA), Rochester, NY.
- April 17, 2020 **20**., Inspection of Excited State Properties in Defected Carbon Nanotubes from Multiple Exciton Generation to Defect-defect Interactions, NDSU Master of Science Thesis Defense Fargo, ND.
- Oct. 14, 2019 19., Interacting Pairs of Surface Defects on Carbon Nanotubes, NDSU Physics Symposium Fargo, ND. Talk
- Aug. 7, 2019 18., Interacting Pairs of Surface Defects on Carbon Nanotubes, Student Symposium, Poster, Los Alamos, NM.
- June 4, 2018 17., Covalent Functionalization of Single-Walled Carbon Nanotubes: Exploring Electronegativity and Steric Effects, Excited State Processes in Electronic and Bio Nanomaterials, Poster, Santa Fe, NM.
- Mar. 8, 2018 **16**., Covalent and non-Covalent Functionalization of Single-Walled Carbon Nanotubes: A MD/DFT Study, APS March Meeting, Poster, Los Angeles, CA.
- Mar. 6, 2018 **15**., Swelling and Structural Properties of Polymer Microgels: Simulations of a Coarse-Grained Model, APS March **Talk** Meeting Los Angeles, CA.
- Feb. 21, 2018 **14**., Covalent Functionalization of Single-Walled Carbon Nanotubes, 58th Annual Sanibel Symposium, Poster, St. Simons Island, GA.
- July 28, 2017 $\mathbf{13}$., Deformation of Single Crystal NiAl and Ni $_3$ Al: A Molecular Dynamics Study, REU Exposition, Poster, Baton Rouge, LA.
- July 21, 2017 12., Deformation of Single Crystal NiAl and Ni₃Al: A Molecular Dynamics Study, CIMM Symposium, Poster, Baton Rouge, LA.
- July 19, 2017 11., Deformation of Single Crystal NiAl and Ni $_3$ Al: A Molecular Dynamics Study, CIMM Symposium: Graduate Invited Talk Student Retreat, New Orleans, LA.
- Nov. 2, 2017 10., Structure and Stability of Colloid-Nanoparticle Suspensions, NDSU Explore Exposition, Poster, Fargo, ND.
- Nov. 2, 2017 **9**., Mixing of Covalent and non-Covalent Functionalization of Carbon Nanotubes, NDSU Explore Exposition, Poster, Fargo, ND.
- Apr. 28, 2017 **8**., Structure and Stability of Colloid-Nanoparticle Suspensions, 2017 Red River Valley Physics & Astrophysics Undergraduate Research Symposium, Poster, Grand Forks, ND.
- Apr. 28, 2017 7., Non-covalent Functionalization of Carbon Nanotubes: Controlling Chirality Selectivity via Alkyl Groups of Conjugated Co-Polymers, 2017 Red River Valley Physics & Astrophysics Undergraduate Research Symposium, Poster, Grand Forks, ND.
- Mar. 18, 2017 6., Structure and Stability of Colloid-Nanoparticle Suspensions, APS March Meeting New Orleans, LA.
- Mar. 17, 2017 **5**., Non-covalent Functionalization of Carbon Nanotubes: Controlling Chirality Selectivity via Alkyl Groups of Conjugated Co-Polymers, APS March Meeting, Poster, New Orleans, LA.
- Feb. 22, 2017 **4.**, Non-covalent Functionalization of carbon Nanotubes: Controlling Chirality Selectivity via Alkyl Groups of Conjugated Co-Polymers, 57th Annual Sanibel Symposium, Poster, St. Simons Island, GA.
- Dec. 15, 2016 3., Non-covalent Functionalization of Carbon Nanotubes: A Study on Binding Energy of Various Branching Positions in Alkyl Groups of Conjugated Co-Polymers, Solving Real-World Problems: An Interdisciplinary Celebration of Research, Poster, Fargo, ND.

- Nov. 2, 2016 **2**., Non-covalent Functionalization of Carbon Nanotubes by Conjugated Co-polymers, NDSU Explore Exposition, Poster, Fargo, ND.
- Apr. 28, 2016 1., Structure and Stability of Colloid-Nanoparticle Suspensions, 2016 Red River Valley Physics & Astrophysics Undergraduate Research Symposium, Poster, Fargo, ND.

References

Dr. Pengfei Huo Assistant Professor of Chemistry Associate Professor of Optics University of Rochester Rochester, NY 14627 1 (585) 276-7793 PENGFEI.HUO@ROCHESTER.EDU

Dr. Svetlana Kilina Assistant Professor of Chemistry North Dakota State University Fargo, ND 58108 1 (701) 231-5622 SVETLANA.KILINA@NDSU.EDU

Dr. Todd Krauss Professor of Chemistry Professor of Optics University of Rochester Rochester, NY 14627 1 (585) 275-5093 TODD.KRAUSS@ROCHESTER.EDU Dr. Sergei Tretiak T-1 Deputy Group Leader Staff Scientist Theoretical Division Los Alamos National Laboratory Los Alamos, NM 87545 1 (505) 667-8351 SERG@LANL.GOV

Dr. Yu Zhang Staff Scientist Theoretical Division Los Alamos National Laboratory Los Alamos, NM 87545 ZHY@LANL.GOV

Dr. Arkajit Mandal Assistant Professor of Chemistry Texas A&M University College Station, TX 77843 1 (585) 770-0424 MANDAL@TAMU.EDU