Braden M. Weight

400 Shady Run Lane Unit 111 Rochester, NY 14625, U.S.A. (701) 202 0603 ⋈ BWEIGHT@UR.ROCHESTER.EDU

Education

2020–Present **Doctor of Philosophy in Physics (Expected Graduation: May 2025)**, *University of Rochester*, Rochester, NY.

2020–2022 **Master of Science in Physics**, *University of Rochester*, Rochester, NY. Cumulative GPA: 3.81/4.00

2018–2020 **Master of Science in Physics**, *North Dakota State University*, Fargo, ND. Cumulative GPA: 4.00/4.00

2014–2018 Bachelor of Science in Physics,
Bachelor of Science in Chemistry,
North Dakota State University, Fargo, ND.
Cumulative GPA: 3.89/4.00

Publications

- Jan. 2023 Braden M. Weight, Todd D. Krauss, and Pengfei Huo. Investigating Molecular Exciton-Polaritons using Many-body Electronic Structure Theory with Cavity Quantum Electrodynamics. University of Rochester, Rochester, NY. In Preparation, ChemRxiv DOI: 10.26434/chemrxiv-2023-2hv8l
- Dec. 2022 Arkajit Mandal,* Michael A.D. Taylor,* **Braden M. Weight**,* Eric R. Koessler,* Xinyang Li, and Pengfei 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 In Revision at *Chemical Reviews* ChemRxiv DOI: 10.26434/chemrxiv-2022-g9Ir7
- Mar. 2023 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. ACS Nano 2023 TBD, 10.1021/acsnano.2c08579
- Jan. 2023 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. Journal of Physical Chemistry Letters, 2023, 14, 5, 1182–1191

 $^{^{}st}$ Authors contributed equally

- Nov. 2022 Deping Hu, Arkajit Mandal, Braden M. Weight, Pengfei Huo. Quasi-Diabatic Propagation Scheme for Simulating Polariton Chemistry. University of Rochester, NY. Journal of Chemical Physics, 157, 194109 (2022)
- August 2022 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.
 Nature Communications 13, 4439 (2022)
 - June 2022 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. Journal of Physical Chemistry Letters 2022, 13, 25, 5801–5807
- August 2021 **Braden M. Weight**, Arkajit Mandal, and Pengfei Huo. *Ab initio* symmetric quasiclassical approach to investigate molecular Tully models. University of Rochester, NY. *Journal of Chemical Physics* 155, 084106 (2021)
- August 2021 **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, NM.

 Journal of Physical Chemistry Letters 2021, 12, 32, 7846–7853
 - Feb. 2021 **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. *Journal of Physical Chemistry C* 2021, 125, 8, 4785–4793
 - Jan. 2021 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. ACS Nano 2021, 15, 1, 923–933
 - Feb. 2020 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. ACS Nano 2020, 14, 3, 3451–3460
 - Nov. 2019 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.

 Nano Letters 2019, 19, 12, 8503-8509

- August 2019 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.

 Journal of Physical Chemistry C 123 (40), 2019, 24807-24817
- March 2018 **Braden M. Weight** and Alan R. Denton, Structure and Stability of Charged Colloid-Nanoparticle Mixtures. Dept. of Physics, North Dakota State University. *Journal of Chemical Physics* **148** (11), 2018, 114904

Presentations

- Mar. 23, 2023 **Braden M. Weight**, Todd D. Krauss, and Pengfei Huo, Investigating Molecular Exciton-Polaritons using Many-body Electronic Structure Theory with Cavity Quantum Electrodynamics.

 APS March Meeting, **Oral Presentation**, Las Vegas, NV
- Feb. 14, 2023 **Braden M. Weight**, Todd D. Krauss, Pengfei Huo, Investigating Molecular Exciton-Polaritons using Many-body Electronic Structure Theory with Cavity Quantum Electrodynamics.

 58th Annual Sanibel Symposium, Poster Presentation, St. Augustine Beach, FL
- Oct. 13, 2022 **Braden M. Weight** and Pengfei Huo, Properties of Molecular Exciton-Polaritons from Simple *ab Initio* Cavity Quantum Electrodynamics Calculations.

 Invited Speaker: North Dakota State University (NDSU) Department of Chemistry and Biochemistry Seminar, Oral Presentation, Fargo, ND
 - Oct. 5, 2022 **Braden M. Weight** and Pengfei Huo, Interfacial Charge Transfer in Rhodamine-based Dye-sensitized TiO2 Quantum Dots with *Ab Initio* Non-adiabatic Excited State Dynamics Simulations.

 ACS North Eastern Regional Meeting (NERM), **Oral Presentation**, Rochester, NY
 - Oct. 4, 2022 **Braden M. Weight** and Pengfei Huo, Properties of Molecular Exciton-Polaritons from Simple *ab Initio* Cavity Quantum Electrodynamics Calculations.

 ACS North Eastern Regional Meeting (NERM), **Oral Presentation**, Rochester, NY
- June. 2, 2022 **Braden M. Weight** and Pengfei Huo, Properties of Molecular Exciton-Polaritons: Coupling *Ab Initio* Calculations with Quantum Optics.

 ACS Middle Atlantic Regional Meeting (MARM), Poster Presentation, Trenton, NJ
- Mar. 23, 2022 **Braden M. Weight** and Pengfei Huo, Properties of Molecular Exciton-Polaritons: Coupling *Ab Initio* Calculations with Quantum Optics.

 University of Rochester Graduate Research Symposium, Poster Presentation, Rochester, NY
- Mar. 14, 2022 **Braden M. Weight** and Pengfei Huo, An On-the-fly Exploration of Recent Spin-based Non-adiabatic Frameworks: spin-LSC and spin-PLDM .

 Invited Speaker Department of Chemistry Poster Session, Poster Presentation, Rochester, NY
- Oct. 21, 2021 **Braden M. Weight**, Andrew E. Sifain, Brendan J. Gifford, Han Htoon, and Sergei Tretiak, 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 (IA) Symposium, Poster Presentation, Rochester, NY

- Sep. 30, 2021 **Braden M. Weight**, Andrew E. Sifain, Brendan J. Gifford, Han Htoon, and Sergei Tretiak, Non-adiabatic Dynamics Simulations of Single-Walled Carbon Nanotubes with Topological sp³-defects: An On-the-fly NEXMD Study .

 Invited Speaker: Virtual International Seminar on Theoretical Advancements (VISTA), Oral Presentation, Rochester, NY
- April 17, 2020 **Braden M. Weight**, Andrew E. Sifain, Brendan J. Gifford, Dmitri Kilin, Svetlana Kilina, Sergei Tretiak, and Andrei Kryjevski, Inspection of Excited State Properties in Defected Carbon Nanotubes from Multiple Exciton Generation to Defect-defect Interactions.

 NDSU Master of Science Thesis Defense, **Oral Presentation**, Fargo, ND
- Oct. 14, 2019 **Braden M. Weight**, Andrew E. Sifain, Brendan J. Gifford, Dmitri Kilin, Svetlana Kilina, Sergei Tretiak, Interacting Pairs of Surface Defects on Carbon Nanotubes. NDSU Physics Symposium, **Oral Presentation**, Fargo, ND
- Aug. 7, 2019 **Braden M. Weight**, Andrew E. Sifain, Brendan J. Gifford, Dmitri Kilin, Svetlana Kilina, Sergei Tretiak, Interacting Pairs of Surface Defects on Carbon Nanotubes. 2019 Student Symposium, Poster Presentation, Los Alamos National Laboratory
- June 4, 2018 **Braden M. Weight**, Brendan J. Gifford, Sergei Tretiak, Svetlana Kilina, Covalent Functionalization of Single-Walled Carbon Nanotubes: Exploring Electronegativity and Steric Effects.

 Excited State Processes in Electronic and Bio Nanomaterials, Poster Presentation, Santa Fe, NM
- Mar. 8 2018 **Braden M. Weight** and Svetlana Kilina, Covalent and non-Covalent Functionalization of Single-Walled Carbon Nanotubes: A MD/DFT Study.

 American Physical Society March Meeting, Poster Presentation, Los Angeles, CA
- Mar. 6 2018 Braden M. Weight and Alan R. Denton, Swelling and Structural Properties of Polymer Microgels: Simulations of a Coarse-Grained Model.
 American Physical Society March Meeting, Oral Presentation, Los Angeles, CA
- Feb. 21 2018 **Braden M. Weight** and Svetlana Kilina, Covalent Functionalization of Single-Walled Carbon Nanotubes.

 58th Annual Sanibel Symposium, Poster Presentation, St. Simons Island, GA
- July 28 2017 **Braden M. Weight** and Juana Moreno, Deformation of Single Crystal NiAl and Ni $_3$ Al: A Molecular Dynamics Study. REU Exposition, Poster Presentation, Baton Rouge, LA
- July 21 2017 **Braden M. Weight** and Juana Moreno, Deformation of Single Crystal NiAl and Ni₃Al: A Molecular Dynamics Study.

 CIMM Symposium, Poster Presentation, Baton Rouge, LA
- July 19 2017 **Braden M. Weight** and Juana Moreno, Deformation of Single Crystal NiAl and Ni₃Al: A Molecular Dynamics Study.

 CIMM Symposium: Graduate Student Retreat, **Oral Presentation**, New Orleans, LA
- Nov. 2 2017 **Braden M. Weight** and Alan R. Denton, Structure and Stability of Colloid-Nanoparticle Suspensions.

 NDSU Explore Exposition, Poster Presentation, Fargo, ND

- Nov. 2 2017 **Braden M. Weight** and Svetlana Kilina, Mixing of Covalent and non-Covalent Functionalization of Carbon Nanotubes.

 NDSU Explore Exposition, Poster Presentation, Fargo, ND
- Apr. 28 2017 **Braden M. Weight** and Alan R. Denton, Structure and Stability of Colloid-Nanoparticle Suspensions.

2017 Red River Valley Physics & Astrophysics Undergraduate Research Symposium, Poster Presentation, Grand Forks, ND

Apr. 28 2017 **Braden M. Weight** and Svetlana Kilina, 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 Presentation, Grand Forks, ND

Mar. 18 2017 **Braden M. Weight** and Alan R. Denton, Structure and Stability of Colloid-Nanoparticle Suspensions.

American Physical Society March Meeting, Poster Presentation, New Orleans, LA

Mar. 17 2017 **Braden M. Weight** and Svetlana Kilina, Non-covalent Functionalization of Carbon Nanotubes: Controlling Chirality Selectivity via Alkyl Groups of Conjugated Co-Polymers.

American Physical Society, Poster Presentation, New Orleans, LA

Feb. 22 2017 **Braden M. Weight** and Svetlana Kilina, Non-covalent Functionalization of carbon Nanotubes: Controlling Chirality Selectivity via Alkyl Groups of Conjugated Co-Polymers.

 57^{th} Annual Sanibel Symposium, Poster Presentation, St. Simons Island, GA

Dec. 15 2016 **Braden M. Weight** and Svetlana Kilina, 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 Presentation, Fargo, ND $\,$

Nov. 2 2016 **Braden M. Weight** and Svetlana Kilina, Non-covalent Functionalization of Carbon Nanotubes by Conjugated Co-polymers.

NDSU Explore Exposition, Poster Presentation, Fargo, ND

Apr. 28 2016 **Braden M. Weight** and Alan R. Denton, Structure and Stability of Colloid-Nanoparticle Suspensions.

2016 Red River Valley Physics & Astrophysics Undergraduate Research Symposium, Poster Presentation, Fargo, ND

Research Experience

2020–Present Research Assistant, Dr. Pengfei Huo, University of Rochester.

Properties of Molecular Exciton-Polaritons: Coupling *Ab Initio* Electronic structure with Quantum Optics,

 Coupling state-of-the-art ab initio quantum chemical calculations with quantum optics exciton-photon interaction models, we successfully model properties of exciton-polaritons to investigate the resulting properties of their strongly correlated wavefunctions.
 In Preparation, ChemRxiv DOI: 10.26434/chemrxiv-2023-2hv8l 2021-Present LANL GRA, Dr. Sergei Tretiak, Los Alamos National Laboratory.

Investigating Resonant Raman Spectroscopy in Functionalized Single-Walled Carbon Nanotubes: An *ab initio* Study,

- Recent experimental results suggest new features in functionalized single-walled carbon nanotubes, which may give functional-specific information.
- Using coupled perturbed Hartree-Fock (CPHF) theory, we compute resonant Raman spectra using perturbation theory at the density functional theory level and make direct comparison to experimental results.

J. Phys. Chem. Lett. 2023, 14, 5, 1182-1191

2020-Present Research Assistant, Dr. Pengfei Huo, University of Rochester.

Asymptotically Decoupled Exciton-Polariton Hamiltonian: Applications to Model Systems in the Reciprocal Space Basis,

Rigorously testing the convergence and applicability of various exciton-polariton Hamiltonians for application to molecular systems, in particular, for use in extended periodic systems in the reciprocal space basis.

Status: In preparation

2020-Present Research Assistant, Dr. Pengfei Huo, University of Rochester.

An On-the-fly Exploration of Recent Spin-based Non-adiabatic Frameworks: spin-LSC and spin-PLDM,

 Investigating the nature of recently developed spin-mapping quantum dynamics methods by direct application to methodologically difficult atomistic model systems, including the sulfur-sulfur bond breaking and re-forming processes in 1,2-dithiane.
 Status: In preparation

2019–2020 LANL GRA, Dr. Sergei Tretiak, Los Alamos National Laboratory.

Interacting Pairs of Surface Defects on Carbon Nanotubes,

Using time-dependent density functional theory (TD-DFT), we model interacting SP³-hybridization defects and fit the interactions to an effective Hamiltonian model of interacting excitons. *J. Phys. Chem. Lett.* 2021, 12, 32, 7846–7853

2019–2020 LANL GRA, Dr. Sergei Tretiak, Los Alamos National Laboratory.

Photoluminescence Dynamics Defined by Exciton Trapping Potential of Coupled Defect-States in DNA-Functionalized Carbon Nanotubes,

- We explained experimental findings of exciton relaxation dynamics based on timedependent density functional theory (TD-DFT) calculations of model systems
- We showed that within a single ssDNA, the defect sites couple strongly through exchange interactions and give rise to an extended exciton trapping potential that houses many dark exciton states and allow for redistribution of exciton population, effectively slowing their relaxation rate.
- In addition, we proved that there exists an J-aggregate-like interaction between extended ssDNA-based exciton trapping potentials, which effectively redistribute the excitonic states, further reducing the excitonic relaxation rate. ACS Nano 2021, 15, 1, 923–933

2018–2020 **Research Assistant**, *Dr. Andrei Kryjevski*, North Dakota State University.

Enhanced Optical Properties of Single-Walled Carbon Nanotubes via SP³-Hybridization Defects from Many-Body Perturbation Theory Based on Density Functional Theory Calculations,

- We employed a novel method based in non-equilibrium, finite-temperature, many-body perturbation theory (MBPT) calculations that utilize output from density functional theory (DFT) to accurately model excited states of these systems
- We solved the Boltzmann transport equation (BE), including phonon absorption/emission
 and biexciton formation/recombination terms to explore phonon-mediated multiple exciton
 generation rates and compute quantum efficiency.

2018–2020 LANL GRA, Dr. Sergei Tretiak, Los Alamos National Laboratory.

Triplet Electronic Configuration in CNTs for Peak Splitting in External Magnetic Fields

- Using the Gaussian package, we explored triplet geometries of CNTs to gauge potential singlet-triplet mixing for various chiralities and configuration positions to assign TDDFT states and explain experimental phenomena.
- I performed all ab initio calculations in this work: ACS Nano 2020, 14, 3, 3451–3460
- 2018–2019 LANL GRA, Dr. Sergei Tretiak, Los Alamos National Laboratory.

Mod(n-m,3) Dependence of Defect-State Emission Bands in Aryl-Functionalized Carbon Nanotubes.

- Using time-dependent density functional theory (TD-DFT), we investigated the relationship between the structural features of sp³-defected carbon nanotubes (CNTs) denoted as (n,m) and the emission energies of various defect configurations and found a direct relationship involving MOD(n-m,3) of the CNT. Nano Letters 2019, 19, 12, 8503-8509
- 2017–2020 Research Assistant, Dr. Svetlana Kilina, North Dakota State University.

Covalent Defects in Carbon Nanotubes: Exploring Redshifts in E^*_{11} by Defect-dependent Charge Localization,

- We characterize the electronic and optical properties of SP³-hybridization defects varying in both orientation about the chiral axis of the carbon nanotube as well as chemical functionality via TD-DFT calculations.
- We utilize the transition density matrix to quantify the effects of these functional groups on the localization of the low-lying excitonic states. J. Phys. Chem. C 2021, 125, 8, 4785–4793
- 2017–2018 Research Assistant, Dr. Alan Denton, North Dakota State University.

Molecular Dynamics Studies on the Structural Response of Colloidal, Cross-linked Polymer Networks to External Stimuli,

- Using a course-grained, atomistic-level model of polymer chains, we explored the validity of the Flory-Rehner theory of polymer swelling implementing the widely-used LAMMPS package.
- 2017 **Research Assistant (NSF REU)**, *Dr. Juana Moreno*, Louisiana State University. (Summer) Molecular Dynamics (MD) Study in Uniaxial Tensile Loading of Binary Alloys,
 - Performed literature review for a deep understanding of the current work and interests in the field of computational and experimental alloy defect mechanisms.
 - o Analyzed stress-strain dependence (Young's Modulus, Poisson's Ratio) on material failure
 - Explored dislocation mechanisms for materials of certain lattice structures (i.e. FCC and BCC) of various Ni-Al crystallographic phases.
- 2015–2019 Research Assistant, Dr. Svetlana Kilina, North Dakota State University.

Molecular Mechanics Studies on Non-Covalent Functionalization of Single-Walled Carbon Nanotubes by Conjugated Co-Polymers,

- Performed classical molecular optimization and dynamics simulations to explore the morphological features of polymer wrapping of carbon nanotubes
- Modified the MM3 parameter set by performing ab initio calculations to extract exact geometric details
- Characterized trends in polymer side chain length and branching as well as trends in carbon nanotube chirality
- A related manuscript was published, where I performed all molecular dynamics simulations and provided support for the main findings in the paper that were computed using only minimization techniques. *Journal of Physical Chemistry C*, 2019, **123**, 40, 24807-24817

- 2015–2018 Research Assistant, Dr. Alan Denton, North Dakota State University.
 - Molecular Dynamics Studies Exploring the Structure and Stability of Colloid-Nanoparticle Suspensions,
 - Illustrated the effects of adding charged nanoparticles to a highly charged suspension of colloidal particles
 - Utilized the Yukawa pair potential to model the screening effect of counterions and salt ions implicitly
 - o Manuscript published in the Journal of Chemical Physics 148 (11), 2018, 114904
- 2015–2016 Research Assistant, Dr. Seth Rasmussen, North Dakota State University.
 - Synthesis of Thiophene-Based Oligomers with Furan Substituents,
 - Performed step-by-step procedures using complex, multi-day synthesis techniques;
 Characterized new, unique compounds utilizing various analysis techniques: Nuclear Magnetic Resonance Spectroscopy, High-Resolution Mass Spectroscopy, Infrared Spectroscopy, UV-VIS Spectroscopy, and Elecrochemistry (Voltammetry)

Teaching Experience

- 2020–2021 **Teaching Assistant Physics**, *University of Rochester*, Rochester, NY.
 - Full-Class Instruction
 - o Facilitate introductory physics-based laboratories at the undergraduate level
 - Coordinate distanced learning through online submission and grading of students' work
- 2018–2020 **Teaching Assistant Physics**, North Dakota State University, Fargo, ND.

Full-Class Instruction

- Taught undergraduate introductory kinematics and electromagnetism laboratories for both upper- (physics majors) and lower- (non-physics majors) level courses
- Learned communication skills needed to address and interact with audiences of varying sizes and backgrounds
- 2018–2020 High School Substitute Teacher, Fargo Public Schools, Fargo, ND.

Full-Class Instruction

- o Certified K-12 license granted by the Education Standards and Practices Board
- Learning communication skills to interact with audiences of varying ages
- Successfully leading large and small group activities
- 2015–2016 **Personal Tutor**, *Self-Employed*, Fargo, ND.

One-on-one Tutoring by Appointment,

- Tutored CHEMISTRY and PHYSICS
- Cultivated different teaching techniques to adapt to various individual learning styles
- Worked through student frustrations by appealing to my own experiences
- Developed independent financial plans for students and worked with individual needs and time constraints
- 2015 **Academic Tutor**, *ACE Tutoring Center, North Dakota State University*, Fargo, ND.

One-on-one and Group Academic Tutoring,

- Tutored MATHEMATICS, CHEMISTRY, PHYSICS, ANTHROPOLOGY, and ENGLISH
- o Developed strong interpersonal skills, increasing my effectiveness as a tutor
- Overcame challenges:
 - Reinforcing students with attempts to inspire creative thinking and personal inquiry
 - Controlling large groups of students by appealing to the overall group's goal of learning
- o Attempted to teach life-long study habits and positive mindsets for the continued success

Computer Skills

Languages: Extensive Experience: Python, Linux, FORTRAN77/95, LaTeX, and Mathematica.

Some Experience: JAVA, C, C++

Packages: SHARC, VASP, GAUSSIAN, MultiWFN, Q-CHEM, LAMMPS, TINKER, VMD,

OVITO, VESTA

Plotting: Origin, Excel, Python/Matplotlib, MATLAB

Computing Extensive experience in high-performance computing: local clusters as well as

national centers (e.g., NERSC)

Honors and Awards

2022 IBM-Zerner Graduate Student Award at the 62th Annual Sanibel Symposium: Quantum Theory Project, St. Augustine Beach, FL

2014-2018 Undergraduate Dean's List

2015–2018 James Sigihara Scholarship for academic excellence, North Dakota State University, Fargo, ND

2018 1^{st} Place Award at the 58^{th} Annual Sanibel Symposium: Quantum Theory Project in the undergraduate poster competition, St. Simons Island, GA

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

2017 North Dakota State University Physics Achievement Award, Fargo, ND

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

Research Interests

Light-Matter Polaritonic chemistry has become the leading direction to control a multitude Interactions 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 excitonic and photonic degrees of freedom hybridize to form new states. These new states can be tuned in various ways to modify and produce unique properties, such as the potential energy landscape or the emission efficiency of materials. These changes will dictate all the resulting properties, such as the absorption/emission spectra and the excited state dynamics.

Quantum The versatility and increasing general interest of nanotechnology is without bound Dynamics and is of great importance to the world. Studying the time-dependence of these Methods 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.

Electronic Electronic properties of materials is a vast and ever-growing realm of research. My Structure ambitions in this field are far-reaching, from molecules to materials, Utilizing excited Theory state theories such as equation of motion coupled cluster to time-dependent density functional theory.

Volunteer Work

- 2019–2020 **Vice President of Graduate Physics Association**, Perform administrative duties that correspond to running a graduate organization, which supports physics students to attend conferences and promotes various outreach activities, 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
- 2016–2020 **Physics Outreach Events**, Physics demos for various activities including elementary schools, community fairs, and other various events , Fargo, ND. 30 Hours
- 2012–2014 **Sanford Health Volunteer**, Aided Sanford Health employees in daily activities mainly stocking, cleaning, and interdepartmental errands, Bismarck, ND. 60 Hours

References

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

Dr. Svetlana Kilina
James A. Meier Professor
Department of Chemistry and Biochemistry
North Dakota State University
Fargo, ND 58108
1 (701) 231-5622
SVETLANA.KILINA@NDSU.EDU

Dr. Sergei Tretiak
Deputy Group Leader of T-1
Staff Scientist Level 5
Center for Integrated Nanotechnologies (CINT)
Los Alamos National Laboratory
Los Alamos, NM 87545
1 (505) 667-8351
SERG@LANL.GOV

Dr. Dmitri Kilin
Assistant Professor
Department of Chemistry and Biochemistry
North Dakota State University
Fargo, ND 58108-6050
1 (206) 356-2212
DMITRI.KILIN@NDSU.EDU