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Braden M. Weight

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.

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.

Preprints and Preparations

TBA **Braden M. Weight*** and Pengfei Huo*. Stochastic Quantum Electrodynamics in the Chebyshev Basis for a Macroscopic Number of Molecules. University of Rochester, Rochester, NY.
In Preparation.

TBA Sanchari Sannigrahi, **Braden M. Weight***, and Pengfei Huo*. Few-molecule Cavity Quantum Electrodynamics Simulations Toward Reactive Pathways and Initial State Preparation. University of Rochester, Rochester, NY.
In Preparation.

May 2024 **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.
In Preparation. ChemRxiv, 2024, DOI: 10.26434/chemrxiv-2024-4hzlj

April 2024 Jialong Wang, **Braden M. Weight***, and Pengfei Huo*. Quantum Electrodynamic Vacuum Fluctuations Influence Chemical Selectivity: A Benchmark and Chemical Explanation. University of Rochester, Rochester, NY.
In Preparation. ChemRxiv, 2024, DOI: 10.26434/chemrxiv-2024-6xsr6-v2

March 2024 **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.
In Review. ChemRxiv, 2024, DOI: 10.26434/chemrxiv-2023-l0lwk

Publications

Mar. 2024 Michael A.D. Taylor*, **Braden M. Weight***, and Pengfei Huo*. Reciprocal Asymptotically Decoupled Hamiltonian for Cavity Quantum Electrodynamics. University of Rochester, Rochester, NY.
Physical Review B, 109, 104305 (2024)

Mar. 2024 **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.
Physical Review A, 109, 032804 (2024)

* Corresponding author

Nov. 2023 **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.
RSC Applied Interfaces, 2024, Advance Article

Sept. 2023 **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.
Physical Chemistry Chemical Physics, 2023, 25, 31554-31577

July 2023 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
Chemical Reviews 2023, 123, 16, 9786–9879

June 2023 **Braden M. Weight**,* Todd D. Krauss, and Pengfei Huo.* Investigating Molecular Exciton Polaritons Using Ab Initio Cavity Quantum Electrodynamics. University of Rochester, Rochester, NY.
Journal of Physical Chemistry Letters 2023, 14, 25, 5901–5913

March 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, 17, 7, 6208–6219

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

Nov. 2022 Deping Hu,* Arkajit Mandal, **Braden M. Weight**, Pengfei Huo.* Quasi-Diabatic Propagation Scheme for Simulating Polariton Chemistry. University of Rochester, 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 quasi-classical approach to investigate molecular Tully models. University of Rochester, 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

† Authors contributed equally

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. 6, 2024 **Braden M. Weight**, Sergei Tretiak, and Yu Zhang, A Diffusion Quantum Monte Carlo Approach to the Polaritonic Ground State.
APS March Meeting, **Oral Presentation**, Las Vegas, NV

Feb. 27, 2024 **Braden M. Weight** and Pengfei Huo, Electrodynamics in the Chebyshev Basis for a Macroscopic Number of Molecules.
63^{th} Annual Sanibel Symposium, Poster Presentation, St. Augustine Beach, FL

Aug. 18, 2023 **Braden M. Weight**, Sergei Tretiak, and Yu Zhang, A Diffusion Quantum Monte Carlo Approach to the Polaritonic Ground State.
LANL Lightning Talk, **Oral Presentation**, Los Alamos, NM

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.
62^{th} 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 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 sp^3-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.
58^{th} 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_3Al: 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 Ni_3Al: 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 Ni_3Al: 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

2023–Present **Research Assistant**, *Dr. Pengfei Huo*, University of Rochester.
Quantum electrodynamic vacuum fluctuations: An *ab initio* study on the nucleophilicity of the bromination of nitrobenzne,

- Developed computational methods to examine the ground state of hybrid exciton-polaritons using the bare electronic density and transition density matrix elements
- Explored the bromination of nitrobenzene and showed that the ground state selectivity can be tuned by the parameters of the optical cavity.
  Status: In preparation

2022–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

2021–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

2022–2023 **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.
  J. Phys. Chem. Lett. 2023, 14, 25, 5901–5913

2021–2023 **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

2021 **Research Assistant**, *Dr. Pengfei Huo*, University of Rochester.
Symmetric Quasi-classical Approach to *ab initio* On-the-fly Dynamics Simulations,
- Investigated the recently suggested *ab initio* Tully models.
- Compared four versions of the state-of-the-art quantum dynamics mapping methods: Symmetric Quasi-classical (SQC) approach.
  J. Chem. Phys. 155, 084106 (2021)

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 SP^3-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 time-dependent 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 SP^3-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 sp^3-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 SP^3-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 (Summer) **Research Assistant (NSF REU)**, *Dr. Juana Moreno*, Louisiana State University.
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.
- 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
- 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

2022–2023 **Introduction to Computational Quantum Mechanics**, Collaboration between University of Rochester (UR) and North Dakota State University (NDSU), Rochester, NY.
- Composed high-level course curriculum, including syllabus, lecture notes, lecture codes, homeworks, and solutions.
- Covered topics include: Python programming, Numerical Calculus, Fourier Analysis, Time-Propagation/Solutions to Ordinary/Partial Differential Equations, Linear Algebra, One-Particle Quantum Mechanics, Mixed Quantum-Classical Dynamics, and Classical and Quantum Monte Carlo Techniques
- Facilitated weekly meetings alternating between lecture-style and homework sessions
- Freely available course materials: Class Website

2020–2021 **Teaching Assistant – Physics**, *University of Rochester*, Rochester, NY.
Full-Class Instruction
- 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
- 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
- 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
- Attempted to teach life-long study habits and positive mindsets for the continued success

Computer Skills

Languages: Extensive Experience: Python, Linux, LaTeX, FORTRAN77/95, and Mathematica.
Some Experience: JAVA, C, C++

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

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

Computing Extensive experience in high-performance computing: local clusters as well as national centers (e.g., NERSC)

Honors and Awards

2023 IBM-Zerner Graduate Student Award at the 62^{th} *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 1^{st} place award in *Solving Real World Problems: Graduate Research Exposition - Interdisciplinary Celebration of Research* for best undergraduate presentation, 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 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 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.

Electronic 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, Utilizing excited state theories such as equation of motion coupled cluster to time-dependent density functional theory as well Monte Carlo approaches.

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

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