

Nadine Claire Bradbury

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Education

University of California, Los Angeles (UCLA)

PhD, Chemistry, Theory and Computation

Oct 2019- Jun 2024

Advisor: Daniel Neuhauser

Thesis: Stochastic Electronic Structure Methods for Nano- to Microscale Molecular Complexes

California Institute of Technology (Caltech)

BSc, Chemistry

Oct 2015 - Jun 2019

Awards & Honors

NSF Graduate Research Fellowship

2021-2024

George Gregory Excellence in Research Award

2023

UCLA Department of Chemistry and Biochemistry

Research Experience

Postdoctoral Research Associate

Sept 2024- Present

Princeton University

Princeton, NJ

- Postdoctoral work with Prof. Joseph Subotnik, on phase space Hamiltonians for inclusion of non-adiabatic effects directly in electronic structure.

Graduate Student Research

Oct 2019 - June 2024

University of California, Los Angeles

Los Angeles, CA

- Novel stochastic electronic structure theory focused on improving the scaling and accuracy of Bethe-Salepeter equation methods.

Undergraduate Senior Thesis

Mar 2018 - Jun 2019

California Institute of Technology

Pasadena, CA

- Advisor: William A Goddard III
- Mechanistic insight into biased versus non-biased ligands for μ -opioid G-protein coupled receptors using molecular dynamics and drug docking softwares.

Caltech Japan Internship Exchange Intern

Jun 2018 - Aug 2018

DiaCel Corporation, Research and Development

Himeji, Hyogo, Japan

Rose Hills Foundation Summer Undergraduate Research Fellowship

Jun 2017 - Aug 2017

California Institute of Technology, Geoffrey Blake Research Group

Pasadena, CA

John Stauffer Summer Undergraduate Research Fellowship

Jun 2016 - Aug 2016

California Institute of Technology, Bill Clemons Research Group

Pasadena, CA

Summer Intern

Jul 2014 - Aug 2014

The Scripps Research Institute, Ardem Patapoutian Group

La Jolla, CA

Summer Intern

Jun 2013 - Aug 2013

The Scripps Research Institute, Ian A Wilson Group

La Jolla, CA

Teaching Assistant Experience

Chemical Thermodynamics	Spring 2021
<i>Chem110a – Evaluations 8.1/9</i>	<i>UCLA</i>
General Chemistry	Fall 2019 - Fall 2020
<i>Chem20ab – Evaluations 8.0/9</i>	<i>UCLA</i>
Nature of the Chemical Bond	Spring 2019
<i>Ch120</i>	<i>Caltech</i>

Research Presentations

Contributed Presentation - ACS Fall 2023	2023
Poster Presentation - ACS Fall 2023	2023
Poster Presentation - ACTC 2022	2022
Poster Presentation - WATOC 2020	2022
Contributed Presentation - ACS Spring 2021	2021

Publications

Peer Reviewed Publications,

- **NC Bradbury**, T Duston, Z Tao, JI Rawlinson, R Littlejohn, JE Subotnik, Symmetry Breaking as Predicted by a Phase Space Hamiltonian with a Spin Coriolis Potential, Submitted (2025). [PDF]
- BY Li, T Duong, T Allen, **NC Bradbury**, JR Caram, D Neuhauser, Parameterized Attenuated Exchange for Generalized TDHF@ v_W Applications, Submitted (2025).[PDF]
- Z Tao, T Qiu, X Bian, T Duston, **NC Bradbury**, JE Subotnik, A basis-free phase space electronic Hamiltonian that recovers beyond Born–Oppenheimer electronic momentum and current density, *J Chem Phys*, 162, 144111 (2025).[PDF]
- J Williams, A Bailey, M Pengshung, AP Deshmukh, C Garcia, J Cao, BY Li, **NC Bradbury**, A Wright, C Chuang, D Neuhauser, E Sletten, JR Caram, Structural Engineering of Cyanine Dyes to Access Highly Redshifted and Emissive J-aggregates. *Chemrxiv*, DOI:10.26434/chemrxiv-2024-k4v5k.
- **NC Bradbury**, BY Li, T Allen, JR Caram, D Neuhauser, No more gap-shifting: Stochastic many-body-theory based TDHF for accurate theory of polymethine cyanine dyes, *J. Chem. Phys.*, 161, 141101 (2024). [PDF]
- **NC Bradbury**, RF Ribeiro, JR Caram, and D Neuhauser, Stochastic methodology shows molecular interactions protect two-dimensional polaritons, *Phys. Rev. B*, 109, L241303 (2024).[PDF]
- M. Sereda, T. Allen, **N. C. Bradbury**, K. Z. Ibrahim, D. Neuhauser Sparse-Stochastic Fragmented Exchange for Large-Scale Hybrid TDDFT Calculations, *J. Chem. Theory Comp.*, 20,10, 4196-4204 (2024) [PDF]
- **NC Bradbury**, T Allen, M Nguyen, and D Neuhauser, Deterministic/Fragmented-Stochastic Exchange for Large Scale Hybrid DFT Calculations, *J. Chem. Theory Comput.*, **19**, 24 (2023). [PDF]

- **NC Bradbury**, M Nguyen, K Ibrahim, and D Neuhauser, Optimized Attenuated Interaction: Enabling Stochastic Bethe-Salpeter Spectra for Large Systems, *J. Chem. Phys.*, **158**, 154104 (2023). [PDF]
- A Bailey, AP Deshmukh, **NC Bradbury**, M Pengshung, T Atallah, J Williams, U Barotov, D Neuhauser, EM Sletten, JR Caram, Exploring the Design of Superradiant J-Aggregates from Amphiphilic Monomer Units, *Nanoscale*, **15**, 3841-3849 (2023). [PDF]
- **NC Bradbury**, M Nguyen, JR Caram, and D Neuhauser, Bethe Salpeter Equation Spectra for Very Large Systems, *J. Chem. Phys.*, **157**, 031104 (2022). [PDF]
- AP Deshmukh, N Geue, **NC Bradbury**, C Chuang, M Pengshung, J Cao, EM Sletten, D Neuhauser, and JR Caram Bridging the gap between H- and J-aggregates: Classification and supramolecular tunability for excitonic band structures in two-dimensional molecular aggregates, *Chem. Phys. Rev.*, **3**, 021401 (2022). [PDF]
- **NC Bradbury**, C Chuang, AP Deshmukh, E Rabani, R Bear, JR Caram, and D Neuhauser, Stochastically Realized Observables for Excitonic Molecular Aggregates. *J. Phys. Chem. A*, **124**, 49, 10111-10120 (2020). [PDF] *Emily Carter Festschrift Invited Paper*

Prior to UCLA,

- A Baranczak, Y Liu, S Connelly, WG Han Du, ER Greiner, JC Genereux, RL Wiseman, YS Eisele, **NC Bradbury**, J Dong, L Noodleman, KB Sharpless, IA Wilson, SE Encalada, and JW Kelly, A Fluorogenic Aryl Fluorosulfate for Intraorganellar Transthyretin Imaging in Living Cells and in *Caenorhabditis elegans*. *JACS*, **137**, **23**, 7404-7414 (2015). [PDF]
- S Connelly, **NC Bradbury**, IA Wilson, High Resolution Structure of Wild Type Human Transthyretin in Complex with 3,3',5,5'-tetrachloro-[1,1'-biphenyl]-4,4'-diol, *RCSB PDB*, **4MAS** (2013).[DOI]