Elizabeth L. Stippell

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EDUCATION

University of Southern California — ***Los Angeles, CA***
PhD Candidate: Physical/Theoretical Chemistry — *08/2021 – Present*
- Oleg Prezhdo group

University at Buffalo — ***Buffalo, NY***
Bachelor of Science, Magna Cum Laude, Chemistry — *08/2017 – 05/2021*
- Minor in Mathematics
- Alexey Akimov group

RESEARCH EXPERIENCE

UNIVERSITY OF SOUTHERN CALIFORNIA

Professor Oleg Prezhdo Research Group — *08/2021 - Present*
- Research focus on a fundamental understanding of energy materials for solar cell design including perovskites and quantum dots using molecular dynamics/non-adiabatic molecular dynamics simulations.
- Mentor to graduate students

LOS ALAMOS NATIONAL LABORATORY

T-1 & T-4 Divisions — *06/2022 – Present*
- Developing machine learning methods to accurately predict and prevent chemical warfare agents
- Constructed a machine learning active learning potential to deepen understanding of nuclear fuels via molecular dynamics simulations

PUBLICATIONS

First Author Publications
- Computational Screening of Ligands for Enhanced Interactions between Lead Halide Perovskite Quantum Dots — *Submitted*
- The Quantum Glissando Effect: Expanding the particle in a box model to include nonadiabatic effects — *In Preparation*
- Employing Fluorine Substitution to Enhance Interlayer Charge Transport in Two-Dimensional Perovskites — *Published 2025*
- Building a DFT+U machine learning interatomic potential for uranium dioxide — *Published 2024*
- Pysycomp: A Symbolic Python Library for the Undergraduate Quantum Chemistry Course — *Published 2023*

Co-Authored Publications
- Mitigating Band Tailing in Kesterite Solar Absorbers: Ab Initio Quantum Dynamics — *Published 2024*
- Self-passivation of Halide Interstitial Defects by Organic Cations in Hybrid Lead-Halide Perovskites: Ab Initio Quantum Dynamics — *Published 2024*
- Nonadiabatic molecular dynamics in Si-nanocrystals in an extended tight-binding framework — *Published 2022*

RESEARCH AWARDS

- Belgian American Educational Foundation Fellowship Recipient — *2023-2024*
- Milligan Fellowship Recipient — *Summer 2021*

UNIVERSITY OF SOUTHERN CALIFORNIA

- Graduate School Fellowship Recipient — *2022 - 2023*

UNIVERSITY AT BUFFALO

- Western New York American Chemical Society Award — *2021*
- American Chemical Society Division of Inorganic Chemistry Award — *2021*
- Provost Scholarship Recipient — *2017 - 2021*
- Albert Padwa Summer Research Award — *Summer 2020*

PRESENTATIONS

- STEMBytes Seminar — *03/2025*
- Virtual International Seminar on Theoretical Advancements (VISTA) — *02/2025*
- Virtual Theoretical Division Lightning Talk Series (Los Alamos National Laboratory) — *07/2023*

WORKSHOPS ATTENDED

- Telluride School on Theoretical Chemistry — *Summer 2025*
- Compchem Cybertraining Workshop — *Summer 2023*
- Libra Winter Workshop — *Winter 2022*
- Compchem Cybertraining Workshop — *Summer 2021*

TEACHING (TA) EXPERIENCE

- CHEM102 (The Molecular World – General Chemistry) — *Fall 2023*
- CHEM115b (Advanced General Chemistry) — *Spring 2022*
- CHEM322a (Organic Chemistry 1) — *Fall 2021*