Elizabeth L. Stippell

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https://liz-stippell.github.io/

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 (Newest to Oldest)

First Author Publications

- The Quantum Glissando Effect: Expanding the particle in a box model to include nonadiabatic effects — *In Preparation*

- **Stippell, E.**; Mora Perez, C.; Favate, N.; Huang, L.; Li, C. W.; Prezhdo, O. V. Computational Screening of Ligands for Enhanced Interactions between Lead Halide Perovskite Quantum Dots. *J. Phys. Chem. Lett.* **2025**, *16* (23), 5666–5673. https://doi.org/10.1021/acs.jpclett.5c01307.

- **Stippell, E.**; Li, W.; Quarti, C.; Beljonne, D.; Prezhdo, O. V. Enhancing Interlayer Charge Transport of Two-Dimensional Perovskites by Structural Stabilization via Fluorine Substitution. *ACS Appl. Mater. Interfaces* **2025**, *17* (1), 2032–2040. https://doi.org/10.1021/acsami.4c17876.

- **Stippell, E.**; Alzate-Vargas, L.; Subedi, K. N.; Tutchton, R. M.; Cooper, M. W. D.; Tretiak, S.; Gibson, T.; Messerly, R. A.

Building a DFT+U Machine Learning Interatomic Potential for Uranium Dioxide. *Artificial Intelligence Chemistry* **2024**, *2* (1), 100042. https://doi.org/10.1016/j.aichem.2023.100042.

- **Stippell, E.**; Akimov, A. V.; Prezhdo, O. V.
  PySyComp: A Symbolic Python Library for the Undergraduate Quantum Chemistry Course. *J. Chem. Educ.* **2023**, *100* (10), 4077–4084. https://doi.org/10.1021/acs.jchemed.2c00974.

Co-Authored Publications

- Anisotropic Exciton-Polariton Relaxation and Phonon Bottleneck in Microcavity-Confined Metal Halide Perovskites: Ab Initio Quantum Dynamics — *In preparation*

- Zhang, P.; **Stippell, E.**; Hou, Z.; Prezhdo, O. V.; Li, W.
  Mitigating Band Tailing in Kesterite Solar Absorbers: Ab Initio Quantum Dynamics.
  J. Am. Chem. Soc. **2024**, *146* (46), 32147–32157. https://doi.org/10.1021/jacs.4c14416.

- Ma, X.; Tian, X.; **Stippell, E.**; Prezhdo, O. V.; Long, R.; Fang, W.-H.
  Self-Passivation of Halide Interstitial Defects by Organic Cations in Hybrid Lead-Halide Perovskites: Ab Initio Quantum Dynamics.
  J. Am. Chem. Soc. **2024**, *146* (42), 29255–29265. https://doi.org/10.1021/jacs.4c12634.

- Shakiba, M.; **Stippell, E.**; Li, W.; Akimov, A. V.
  Nonadiabatic Molecular Dynamics with Extended Density Functional Tight-Binding: Application to Nanocrystals and Periodic Solids.
  J. Chem. Theory Comput. **2022**, *18* (9), 5157–5180. https://doi.org/10.1021/acs.jctc.2c00297.

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

- The American Chemical Society (ACS) Fall 2025 Conference: Energy and Fuels Division — *08/2025*

- The American Chemical Society (ACS) Fall 2025 Conference: Physical Chemistry Division — *08/2025*
- USC Women in Science and Engineering 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*