

Sarah Allec

Postdoctoral Research Associate

Contact

Address

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Skills

Research

Interdisciplinary
Coordination

Python and C++ proficiency

Highly motivated postdoctoral researcher with experience in computational chemistry and materials science, data science, and high-performance computing. Has research and course experience in C++ and Python programming languages, as well as a variety of computational chemistry/materials science programs (e.g., VASP, SIESTA, CP2K, LAMMPS). Passionate about collaborative and interdisciplinary research and development.

Employment History

2020-09 -
Current

Postdoctoral Research Associate

Pacific Northwest National Laboratory, Richland, WA

- Conduct research on the computational design and modeling of carbon capture solvents and surface catalysts using ab initio molecular dynamics, quantum chemical methods, and machine learning.
- Collaborate with team members as well as with multidisciplinary research groups at PNNL and universities.
- Write and publish peer-reviewed articles concerning findings and highlight possible applications for findings.

Education

2018-09 -
2020-09

Ph.D.: Materials Science & Engineering, Computational Materials Science & Engineering

University of California Riverside

GPA: 3.96, Advisor: P. Alex Greaney

2015-09 -
2018-09

M.S.: Materials Science & Engineering, Computational Materials Science & Engineering

University of California Riverside

GPA: 3.96, Advisor: Bryan M. Wong

2011-09 -
2015-06

B.S.: Mathematics, Physics

University of California Riverside

GPA: 3.97, Graduated summa cum laude

Selected Publications

- Sarah I. Allec, Melissa T. Manetsch, Loukas Kollias, *et al.*, "Data Science Driven CO₂ Diels Alder reactions: Novel pathways for CO₂ Bond Activation and Conversion", *in submission process*.
- Loukas Kollias, Difan Zhang, Sarah I. Allec, *et al.*, "Advanced Theory and Simulation to Guide the Development of CO₂ Capture Solvents." *ACS Omega*, **7**, 12453-12466 (2022).
- Sarah I. Allec, Manh-Thuong Nguyen, Roger Rousseau, and Vassiliki-Alexandra Glezakou, "The Role of Sub-Surface Hydrogen on CO₂ Reduction and Dynamics on Ni(110): An Ab Initio Molecular Dynamics Study." *Journal of Chemical Physics*, **155**, 044702 (2021).

Awards/Grants

- NERSC ERCAP Award (306,500 CPU hours), PNNL, 2022
- NSF Graduate Research Fellowship, UC Riverside 2017
- NASA MIRO FIELDS Graduate Student Fellowship

Volunteer Experience

- Association for Women in Science, UCR, Co-President, 2019-2020
- Association for Women in Science, UCR, Treasurer, 2018-2019
- School on Wheels Tutor, 2018 – Present
- FIRST LEGO League Coach, 2015-2016