Sarah I. Allec

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EDUCATION

University of California Riverside

Ph.D. in Materials Science & Engineering, 3.96 GPA 2020

Concentration: Computational Materials Science & Engineering

Thesis: Atomistic modeling of amorphous materials

Advisor: Dr. P. Alex Greaney

B.S. in Mathematics (Applied), 3.97 GPA, *Summa cum laude* 2015

Concentration: Physics

EMPLOYMENT

Citrine Informatics 2022-Present

Research Scientist II

Supervisor: Dr. James Saal

Pacific Northwest National Laboratory 2020-2022

Postdoctoral Research Associate

Supervisor: Dr. Roger Rousseau

PUBLICATIONS

Eric D. Walter, Difan Zhang, Ying Chen, Kee Sung Han, J. David Bazak, Sarah Burton, Kathryn O'Harra, David W. Hoyt, Jason E. Bara, Deepika Malhotra, **Sarah I. Allec**, Vassiliki-Alexandra Glezakou, David J. Heldebrant, and Roger Rousseau, "Enhancing CO_2 Transport Across a PEEK-Ionene Membrane and Water-Lean Solvent Interface." *ChemSusChem*, **16**, e202300157 (2023).

Linxiao Chen, **Sarah I. Allec**, Manh-Thuong Nguyen, Libor Kovarik, Adam S. Hoffman, Jiyun Hong, Debora Meira, Honghong Shi, Simon R. Bare, Vassiliki-Alexandra Glezakou, Roger Rousseau, and János Szanyi, "Dynamic Evolution of Palladium Single Atoms on Anatase Titania Support Determines the Reverse Water–Gas Shift Activity." *Journal of the American Chemical Society*, **145**, 10847-10860 (2023).

Runze Ma, Christopher R. O'Connor, Gregory Collinge, **Sarah I. Allec**, Mal-Soon Lee, and Zdenek Dohnálek, "The Role of Surface Hydroxyls in the Mobility of Carboxylates on Surfaces: Dynamics of Acetate on Anatase TiO_2(101)." *The Journal of Physical Chemistry Letters*, **14**, 2542-2550 (2023).

Loukas Kollias, Difan Zhang, **Sarah I. Allec**, Manh-Thuong Nguyen, Mal-Soon Lee, David C. Cantu, Roger Rousseau, and Vassiliki-Alexandra Glezakou, "Advanced Theory and Simulation to Guide the Development of CO_2 Capture Solvents." *ACS Omega*, **7**, 12453-12466 (2022).

Loukas Kollias, Gregory Collinge, Difan Zhang, **Sarah I. Allec**, Pradeep Kumar Gurunathan, GiovanniMaria Piccini, Simuck F. Yuk, Manh-Thuong Nguyen, Mal-Soon Lee, Vassiliki-Alexandra Glezakou, and Roger Rousseau, "Assessing entropy for catalytic processes at complex reactive interfaces." *Annual Reports in Computational Chemistry*, **18**, 3-51 (2022).

Manh-Thuong Nguyen, Katarzyna Grubel, Difan Zhang, Phillip K. Koech, Deepika Malhotra, **Sarah Allec,** Roger Rousseau, Vassiliki-Alexandra Glezakou, and David J. Heldebrant, "Amphilic Water-Lean Carbon Capture Solvent Wetting Behavior through Decomposition by Stainless-Steel Interfaces." *ChemSusChem*, **14**, 5283 (2022).

Sarah I. Allec, Manh-Thuong Nguyen, Roger Rousseau, and Vassiliki-Alexandra Glezakou, "The Role of Sub-Surface Hydrogen on CO_2 Reduction and Dynamics on Ni(110): An Ab Initio Molecular Dynamics Study." Journal of Chemical Physics, 155, 044702 (2021).

Jon M. Matxain, Jesus M. Ugalde, Vladimiro Mujica, **Sarah I. Allec**, Bryan M. Wong, and David Casanova, "Chirality Induced Spin Selectivity of Photoexcited Electrons in Carbon-Sulfur [*n*]Helicenes." *ChemPhotoChem*, **3**, 770-777 (2019).

Sarah I. Allec, Yijing Sun, Jianan Sun, Chia-en A. Chang, and Bryan M. Wong, "Heterogeneous CPU+GPU-Enabled Simulations for DFTB Molecular Dynamics of Large Chemical and Biological Systems." *Journal of Chemical Theory and Computation*, **15**, 2807-2815 (2019).

Sarah I. Allec, Anshuman Kumar, and Bryan M. Wong, "Linear-Response and Real-Time, Time-Dependent DFT for Predicting Optoelectronic Properties of Dye-Sensitized Solar Cells." *Dye Sensitized Solar Cells*, 171-201 (2019).

Yue Cao, Haiping Wu, **Sarah I. Allec**, Bryan M. Wong, Dai-Scott Nguyen, and Chao Wang, "A Highly Stretchy, Transparent Elastomer with the Capability to Automatically Self-Heal Underwater." *Advanced Materials*, **30**, 1804602 (2018).

Yue Cao, Timothy G. Morrissey, Eric Acome, **Sarah I. Allec**, Bryan M. Wong, Christoph Keplinger, and Chao Wang, "A Transparent, Self-Healing, Highly Stretchable Ionic Conductor." *Advanced Materials*, **29**, 1605099 (2017).

Sarah I. Allec and Bryan M. Wong, "Inconsistencies in the Electronic Properties of Phosphorene Nanotubes: New Insights from Large-Scale DFT Calculations." *Journal of Physical Chemistry Letters,* **7**, 4340-4345 (2016).

Sarah I. Allec, Niranjan V. Ilawe, and Bryan M. Wong, "Unusual Bandgap Oscillations in Template-Directed π -Conjugated Porphyrin Nanotubes." *Journal of Physical Chemistry Letters*, **7**, 2362-2367 (2016).

AWARDS

NSF Graduate Research Fellowship, UC Riverside 2017

NASA MIRO FIELDS Graduate Student Fellowship, UC Riverside 2016

FUNDED GRANTS

National Energy Research Scientific Computing Center (NERSC) ERCAP Award 2022

Computational Screening of Redox couples for the Direct Air Capture Of CO_2 via Electrochemical pH swing, 306,500 CPU hours and 800 GPU hours

LEADERSHIP EXPERIENCE

AWIS UCR Co-President 2019-2020

Set goals, vision, and direction for AWIS UCR

AWIS UCR Treasurer 2018-2019

Managed organization's finances through budgeting and allocation of funds

School on Wheels Tutor 2018-2021

Serve as a positive role model to provide consistency and educational assistance to homeless students in Riverside

Supplemental Instruction Mentor, UC Riverside Academic Resource Center 2014-2015

Mentored a group of 7 Supplemental Instruction Leaders and organized new employee training

Supplemental Instruction Leader, UC Riverside Academic Resource Center 2013-2015

Facilitated weekly study sessions for historically difficult courses