Sarah 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

Advisor: Dr. P. Alex Greaney

M.S. in Materials Science & Engineering, 3.96 GPA 2018

Concentration: Computational Materials Science & Engineering

Advisor: Dr. Bryan M. Wong

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

Concentration: Physics

EMPLOYMENT

Citrine Informatics 2022 - Present

Research Scientist

Supervisor: James Saal

Pacific Northwest National Laboratory 2020 - 2022

Postdoctoral Research Associate

Supervisor: Marat Valiev

PUBLICATIONS

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).

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).

Chong Zhang, Woochul Shin, Liangdong Zhu, Cheng Chen, Joerg C. Neuefeind, Yunkai Xu, Sarah I. Allec, Cong Liu, Zhixuan Wei, Aigerim Daniyar, Jia-Xing Jiang, Chong Fang, P. Alex Greaney, and Xiulei Ji, "The Electrolyte Comprising More Robust Water and Superhalides Transforms Zn-Metal Anode Reversibly and Dendrite-Free." *Carbon Energy*, **3**, 339-348 (2020).

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

OUTREACH

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-Present

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

FIRST LEGO League Coach 2015-2016

Mentored a group of 7 middle school students in robot design and programming