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

Pacific Northwest National Laboratory 2020 - Present

Postdoctoral Research Associate

Supervisor: Roger Rousseau

PUBLICATIONS

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

PRESENTATIONS

TMS2020 Annual Meeting & Exhibition 2020
Neural Network Potentials for Water-in-Salt Electrolytes

MRS Spring Meeting 2019 2019
Silicon-Based Spintronics: Experimental and Theoretical Validation of Spin Manipulation in Silicon

MRS Spring Meeting 2018 2018
Large-Scale DFT Calculations for the Discovery of Novel Nanotubes

APS March Meeting 2018 2018
Large-Scale DFT Calculations for the Discovery of Novel Nanotubes

253rd ACS National Meeting 2017
GPU-Enabled Real-Time Electron Dynamics of Nitrogen-Doped Graphene Nanoflakes

ASM International Meeting, San Fernando Valley Chapter 2017
Electronic Properties of Nanomaterials: A Quantum Mechanical Perspective

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