

# 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:* R. Scott Smith

## 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<sub>2</sub> 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<sub>2</sub> 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, Niranjana V. Ilawe, and Bryan M. Wong, "Unusual Bandgap Oscillations in Template-Directed  $\pi$ -Conjugated Porphyrin Nanotubes." *Journal of Physical Chemistry Letters*, **7**, 2362-2367 (2016).

## AWARDS

<i>NSF Graduate Research Fellowship</i> , UC Riverside	2017
<i>NASA MIRO FIELDS Graduate Student Fellowship</i> , UC Riverside	2016

## FUNDED GRANTS

National Energy Research Scientific Computing Center (NERSC) ERCAP Award <i>Computational Screening of Redox couples for the Direct Air Capture Of CO<sub>2</sub> via Electrochemical pH swing</i> , 306,500 CPU hours and 800 GPU hours	2022
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## PRESENTATIONS

TMS2020 Annual Meeting & Exhibition <i>Neural Network Potentials for Water-in-Salt Electrolytes</i>	2020
MRS Spring Meeting 2019 <i>Silicon-Based Spintronics: Experimental and Theoretical Validation of Spin Manipulation in Silicon</i>	2019
MRS Spring Meeting 2018 <i>Large-Scale DFT Calculations for the Discovery of Novel Nanotubes</i>	2018
APS March Meeting 2018 <i>Large-Scale DFT Calculations for the Discovery of Novel Nanotubes</i>	2018
253 <sup>rd</sup> ACS National Meeting <i>GPU-Enabled Real-Time Electron Dynamics of Nitrogen-Doped Graphene Nanoflakes</i>	2017
ASM International Meeting, San Fernando Valley Chapter <i>Electronic Properties of Nanomaterials: A Quantum Mechanical Perspective</i>	2017

## OUTREACH

AWIS UCR Co-President Set goals, vision, and direction for AWIS UCR	2019-2020
AWIS UCR Treasurer Managed organization's finances through budgeting and allocation of funds	2018-2019

**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