

Sarah Allec

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SUMMARY

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

EMPLOYMENT

Citrine Informatics

2022 - Present

Research Scientist

Supervisor: James Saal

- Perform research in materials informatics for a variety of applications and material domains
- Engage with collaborators at universities, national laboratories, and other companies
- Aid in the preparation of responses to requests for proposals (RFPs)
- Publish technical work in peer-reviewed journal articles, case studies, and blog posts

Pacific Northwest National Laboratory

2020 - 2022

Postdoctoral Research Associate

Supervisor: Marat Valiev

- Conducted research on the computational design and modeling of carbon capture solvents and surface catalysts using *ab initio* molecular dynamics and density functional theory
- Collaborated with team members as well as with multidisciplinary research groups at PNNL and universities
- Wrote and published peer-reviewed journal articles concerning research findings

EDUCATION

University of California Riverside

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

2020

Concentration: Computational Materials Science & Engineering

Advisor: P. Alex Greaney

M.S. in Materials Science & Engineering, 3.96 GPA	2018
<i>Concentration:</i> Computational Materials Science & Engineering	
<i>Advisor:</i> Bryan M. Wong	
B.S. in Mathematics (Applied), 3.97 GPA, <i>Summa cum laude</i>	2015
<i>Concentration:</i> Physics	

LEADERSHIP EXPERIENCE

Association for Women in Science, UC Riverside: Co-President	2019-2020
<ul style="list-style-type: none"> • Set goals, vision, and direction for AWIS UCR • Lead all general and board meetings • Serve as official representative within and outside of UCR 	
Association for Women in Science, UC Riverside: Treasurer	2018-2019
<ul style="list-style-type: none"> • Maintained AWIS UCR's finances through budgeting and allocation of general funds • Secured \$2000 sponsorship from UCR's Dean of the College of Natural & Agricultural Sciences for networking brunch 	
FIRST LEGO League Coach	2015-2016
<ul style="list-style-type: none"> • Coached a team of 5 middle school students in LEGO robot design, programming, and teamwork • Taught a corresponding robotics class for homeschooled students 	
UCR Academic Resource Center: Supplemental Instruction Mentor	2014-2015
<ul style="list-style-type: none"> • Mentored a group of 7 SI Leaders • Organized and facilitated SI Leader training 	
UCR Academic Resource Center: Supplemental Instruction Leader	2013-2015
<ul style="list-style-type: none"> • Facilitated weekly study sessions in historically difficult courses • Collaborated with UCR faculty 	

VOLUNTEER EXPERIENCE

School on Wheels Tutor	2018-Present
<ul style="list-style-type: none"> • Tutor and mentor homeless students on a weekly basis in all subjects • Monitor grades of student and communicate with teachers regarding progress • Act as a positive and supportive role model for students 	