

Sarah Allec

Research Scientist

Researcher in *in-silico materials design*, combining *state-of-the-art physics-based modeling and data science techniques* to design new materials.



sarah.allec@gmail.com



(951)217-1971



Boise, ID, United States



sarah-allec.github.io/



linkedin.com/in/sarah-allec



github.com/sarah-allec

EDUCATION

Ph.D., Materials Science & Engineering

University of California Riverside

09/2015 - 09/2020

3.97 GPA

Thesis

- Atomistic Modeling of Amorphous Materials

B.S., Applied Mathematics (Physics)

University of California Riverside

09/2011 - 06/2015

Summa cum laude

SKILLS

Density functional theory

Molecular dynamics

Machine learning

SQL

UI

Python

Linux

PROFESSIONAL EXPERIENCE

Research Scientist II

Citrine Informatics

10/2022 - Present

Citrine Informatics is the world leader in generative AI for materials and chemicals product development.

Tasks

- Perform cutting-edge research in **materials informatics**.
- Manage technical aspects of funded programs.
- Collaborate with researchers** at universities, national labs, and other companies.
- Aid in the **preparation of responses to requests for proposals** (RFPs).

Contact : James E. Saal - jsaal@citrine.io

Remote

Postdoctoral Research Associate

Pacific Northwest National Laboratory

09/2020 - 09/2022

PNNL is a leading center for scientific discovery in chemistry, data analytics, Earth science, sustainable energy, and national security.

Thesis

- Performed research on the computational design of carbon capture solvents and catalysts using **ab initio molecular dynamics and density functional theory**.
- Collaborated with team members** in multidisciplinary research groups.
- Published peer-reviewed journal articles** concerning research findings.

Contact : Marat Valiev - marat.valiev@pnl.gov

Richland, WA

PUBLICATIONS

Invited manuscript

Evaluation of GlassNet for physics-informed machine learning of glass stability and glass-forming ability

Author(s)

Sarah I. Allec, Xiaonan Lu, Daniel R. Cassar, Xuan T. Nguyen, Vinay I. Hegde, Thiruvillamalai Mahadevan, Miroslava Peterson, Jincheng Du, Brian J. Riley, John D. Vienna, James E. Saal

2024, Submitted

Journal of the American Ceramic Society

A pre-print is available on arXiv: <https://doi.org/10.48550/arXiv.2403.10682>

Research article

A case study of multimodal, multi-institutional data management for the combinatorial materials science community

Author(s)

Sarah I. Allec, Eric S. Muckley, Nathan S. Johnson, Christopher K. H. Borg, Dylan J. Kirsch, Joshua Martin, Rohit Pant, Ichiro Takeuchi, Andrew S. Lee, James E. Saal, Logan Ward, Apurva Mehta

2024, Accepted

Integrating Materials and Manufacturing Innovation

A pre-print is available on arXiv: <https://doi.org/10.48550/arXiv.2311.10205>

COMPUTING RESOURCES

Director Reserve Award
(01/2024 - Present)

National Energy Research Scientific Computing Center (NERSC)

- 10,000 CPU hours and 100 GPU hours for the application of active machine learning to nuclear waste form design

DOE Mission Science Award
(01/2022 - 12/2023)

National Energy Research Scientific Computing Center (NERSC)

- 306,500 CPU hours and 800 GPU hours for the computational screening of redox couples for the electrochemical direct Air Capture of CO₂

PEER REVIEW

DOE Office of Science
SBIR/STTR Proposal
Reviewer (12/2023)

Royal Society of Chemistry
(RSC) Digital Discovery Peer
Reviewer (01/2024)

AWARDS

NSF Graduate Research
Fellowship (2017 - 2020)

NASA MIRO FIELDS
Graduate Student Fellowship
(2016 - 2017)

MENTORSHIP

Undergraduate Mentor
Cal Poly San Luis
Obispo Materials
Engineering (MATE)
Summer Research
Program

07/2023 - 09/2023
Remote

Graduate Intern Mentor
DOE Office of Science,
Science Undergraduate
Laboratory Internships
(SULI) Program

06/2021 - 09/2021
Richland, WA

PUBLICATIONS

Research article

Tetrameric Self-assembly of Water-Lean Solvents enables carbamate anhydride-based CO₂ capture Chemistry

Author(s)

Julien Leclaire, David J. Heldebrant, Katarzyna Grubel, Jean Septavaux, Marc Hennenbelle, Eric Walter, Ying Chen, Jose Leobardo Bañuelos, Difan Zhang, Manh Thuong Ngyuen, Debmalya Ray, Sarah Allec, Deepika Malhotra, Wontae Joo, Jaelynn King

2024, Accepted

Nature Chemistry

Research article

Enhancing CO₂ Transport Across a PEEK-Ionene Membrane and Water-Lean Solvent Interface

Author(s)

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, Roger Rousseau

2023, Published

ChemSusChem, 16, e202300157

<https://doi.org/10.1002/cssc.202300157>

Research article

Dynamic Evolution of Palladium Single Atoms on Anatase Titania Support Determines the Reverse Water-Gas Shift Activity

Author(s)

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, János Szanyi

2023, Published

Journal of the American Chemical Society, 145, 10847-10860

<https://doi.org/10.1021/jacs.3c02326>

Research article

The Role of Surface Hydroxyls in the Mobility of Carboxylates on Surfaces: Dynamics of Acetate on Anatase TiO₂(101)

Author(s)

Runze Ma, Christopher R. O'Connor, Gregory Collinge, Sarah I. Allec, Mal-Soon Lee, Zdenek Dohnálek,

2023, Published

Journal of Physical Chemistry Letters, 14, 2542-2550

<https://doi.org/10.1021/acs.jpcllett.3c00175>

Perspective article

Advanced Theory and Simulation to Guide the Development of CO₂ Capture Solvents

Author(s)

Loukas Kollias, Difan Zhang, Sarah I. Allec, Manh-Thuong Nguyen, Mal-Soon Lee, David C. Cantu, Roger Rousseau, Vassiliki-Alexandra Glezakou

2022, Published

ACS Omega, 7, 12453-12466

<https://doi.org/10.1021/acsomega.1c07398>

Book chapter

Assessing entropy for catalytic processes at complex reactive interfaces

Author(s)

Loukas Kollias, Gregory Collinge, Difan Zhang, Sarah I. Allec, Pradeep Kumar Gurunathan, Giovanni Maria Piccini, Simuck F. Yuk, Manh-Thuong Nguyen, Mal-Soon Lee, Vassiliki-Alexandra Glezakou, Roger Rousseau

2022, Published

Annual Reports in Computational Chemistry, 18, 3-51

<https://doi.org/10.1016/bs.arcc.2022.09.004>

INVITED TALKS

Novel approaches to informatics-driven nuclear waste form design: Dataset curation, surrogate modeling, and sequential learning (05/2024)

ACerS Glass & Optical Materials Division (GOMD) Meeting 2024

OUTREACH

Community Volunteer Interfaith Sanctuary

2023 - Present

Boise, ID

Greet and check in guests, support shelter operations, data management

Workshop Leader Citrine Informatics

2023

San Luis Obispo, CA

Led a workshop for educators at the North American Materials Education Symposium

Co-President

Association for Women in Science, UC Riverside Chapter

2019 - 2020

Riverside, CA

Set goals, vision, and direction; hosted outreach and fundraising events

Treasurer

Association for Women in Science, UC Riverside Chapter

2018 - 2019

Riverside, CA

Managed finances through budgeting and allocation of funds

Mentor/Tutor School on Wheels

2018 - 2021

Riverside, CA

Mentored and tutored homeless students in southern California

PUBLICATIONS

Research article

Amphiphilic Water-Lean Carbon Capture Solvent Wetting Behavior through Decomposition by Stainless-Steel Interfaces

Author(s)

Manh-Thuong Nguyen, Katarzyna Grubel, Difan Zhang, Phillip K. Koech, Deepika Malhotra, Sarah Allec, Roger Rousseau, Vassiliki-Alexandra Glezakou, David J. Heldebrant

2022, Published

ChemSusChem, 14, 5283

<https://doi.org/10.1002/cssc.202101350>

Research article

The Role of Sub-Surface Hydrogen on CO₂ Reduction and Dynamics on Ni(110): An Ab Initio Molecular Dynamics Study

Author(s)

Sarah I. Allec, Manh-Thuong Nguyen, Roger Rousseau, Vassiliki-Alexandra Glezakou

2021, Published

Journal of Chemical Physics, 155, 044702

<https://doi.org/10.1063/5.0048894>

Research Article

The electrolyte comprising more robust water and superhalides transforms Zn-metal anode reversibly and dendrite-free

Author(s)

Chong Zhang, Woochul Shin, Liangdong Zhu, Cheng Chen, Joerg C. Neufeind, Yunkai Xu, Sarah I. Allec, Cong Liu, Zhixuan Wei, Aigerim Daniyar, Jia-Xing Jiang, Chong Fang, P. Alex Greaney, Xiulei Ji

2021, Published

Carbon Energy, 3, 339-348

<https://doi.org/10.1002/cey2.70>

Research article

Chirality Induced Spin Selectivity of Photoexcited Electrons in Carbon-Sulfur [n]Helicenes

Author(s)

Jon M. Matxain, Jesus M. Ugalde, Vladimiro Mujica, Sarah I. Allec, Bryan M. Wong, David Casanova

2019, Published

ChemPhotoChem, 3, 770-777

<https://doi.org/10.1002/cptc.201900128>

Research article

Heterogeneous CPU+GPU-Enabled Simulations for DFTB Molecular Dynamics of Large Chemical and Biological Systems

Author(s)

Sarah I. Allec, Yijing Sun, Jianan Sun, Chia-en A. Chang, Bryan M. Wong

2019, Published

Journal of Chemical Theory and Computation, 15, 2807-2815

<https://doi.org/10.1021/acs.jctc.8b01239>

Book chapter

Linear-Response and Real-Time, Time-Dependent DFT for Predicting Optoelectronic Properties of Dye-Sensitized Solar Cells

Author(s)

Sarah I. Allec, Anshuman Kumar, Bryan M. Wong

2019, Published

Dye-Sensitized Solar Cells, 171-201

<https://doi.org/10.1016/B978-0-12-814541-8.00005-7>

OUTREACH

Supplemental Instruction Mentor

UC Riverside Academic
Resource Center

2014 - 2015

Riverside, CA

Mentored Supplemental Instruction
Leaders and organized training

Supplemental Instruction Leader

UC Riverside Academic
Resource Center

2013 - 2015

Riverside, CA

Facilitated weekly group tutoring sessions
for historically difficult courses

REFERENCES

James E. Saal

jsaal@citrine.io - (847) 425-8233

David J. Heldebrant

david.heldebrant@pnnl.gov -
(509) 372-6359

P. Alex Greaney

peter.greaney@ucr.edu - (951) 827-2884

PUBLICATIONS

Research article

A Highly Stretchy, Transparent Elastomer with the Capability to Automatically Self-Heal Underwater

Author(s)

Yue Cao, Haiping Wu, Sarah I. Allec, Bryan M. Wong, Dai-Scott Nguyen, Chao Wang

2018, *Published*

Advanced Materials, 30, 1804602

<https://doi.org/10.1002/adma.201804602>

Research article

A Transparent, Self-Healing, Highly Stretchable Ionic Conductor

Author(s)

Yue Cao, Timorothy G. Morrissey, Eric Acome, Sarah I. Allec, Bryan M. Wong, Christoph Keplinger, Chao Wang

2017, *Published*

Advanced Materials, 29, 1605099

<https://doi.org/10.1002/adma.201605099>

Research article

Inconsistencies in the Electronic Properties of Phosphorene Nanotubes: New Insights from Large-Scale DFT Calculations

Author(s)

Sarah I. Allec, Bryan M. Wong

2016, *Published*

Journal of Physical Chemistry Letters, 7, 4340-4345

<https://doi.org/10.1021/acs.jpcllett.6b02271>

Research article

Unusual Bandgap Oscillations in Template-Directed π -Conjugated Porphyrin Nanotubes

Author(s)

Sarah I. Allec, Niranjan V. Ilawe, Bryan M. Wong

2016, *Published*

Journal of Physical Chemistry Letters, 7, 2362-2367

<https://doi.org/10.1021/acs.jpcllett.6b01020>