

Curriculum Vitae

Personal Information

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Education

Doctor of Philosophy in Chemical Engineering, 2019 – University of California, Los Angeles

Bachelor of Science in Chemical Engineering, 2013 – California State University, Long Beach
Bachelor of Arts in Chemistry, 2013 – California State University, Long Beach

Professional Experience

OAK RIDGE NATIONAL LABORATORY, Oak Ridge, TN

Research Scientist, January 2021 – Present

Research combining machine learning with computational chemistry methods for materials discovery and theory-experiment matching in the Center for Nanophase Materials Sciences.

MITRE CORPORATION, McLean, VA

Senior Modeling & Simulation Engineer/Analyst, August 2019 – January 2021

Computational researcher using physics-based modeling, simulation, machine learning, & analysis to deliver meaningful solutions to national security challenges related to materials science, electro-optics, & systems engineering.

LOS ALAMOS NATIONAL LABORATORY, Los Alamos, NM

African American Partnership Program (AAPP) Fellow, August 2015 – June 2019

Graduate student researcher using advanced materials characterization, electrochemistry, ultrafast laser spectroscopy, and modeling/simulation methods to resolve material-structure-property relationships.

UNIVERSITY OF CALIFORNIA LOS ANGELES, Los Angeles, CA

Graduate Student Researcher, September 2013 – June 2019

Graduate student researcher using experimental and computational (density functional theory) methods to study nanomaterials & porous materials for energy storage, energy harvesting, & catalysis applications.

CALIFORNIA STATE UNIVERSITY LONG BEACH, Long Beach, CA

Undergraduate Student Researcher, January 2011 – September 2013

Undergraduate student researcher using synthetic chemistry and X-ray crystallography methods to synthesize new porous materials for carbon capture and ion-exchange membranes.

Awards

- Weinberg Distinguished Staff Fellowship (**Oak Ridge National Laboratory**, 2021-2024)
- Catalyst Award (**MITRE**, July 2020)
- Three Spark Awards (**MITRE**, February 2020, April 2020, September 2020)
- Three ROAR Awards (**MITRE**, June 2020, July 2020, August 2020)
- Leveraged Project Success Story (**New Mexico Small Business Association**, or **NMSBA**, 2017)
- Ben Lujan Small Business Excellence Award (**NMSBA**, 2017)
- African American Partnership Program (AAPP) Fellowship (**Los Alamos National Laboratory**, 2015 – 2019)
- Green Energy Undergraduate Student Poster Award (**IEEE**, 2013)
- RISE Fellowship (**NIH**, 2012-2013)

Publications & Patents

Google Scholar: <https://scholar.google.com/citations?user=4z1E-HEAAAAJ&hl=en>

- *Patents:*
 1. Cai, M.; Lu, Y.; Yang, L.; Fang, D.; Shen, J.; **Fuhr, A.**; Shen, L. (2018). “Electrolyte Structure for Metal Batteries”, US Patent number 20160254567A1
- *Publications:*
 1. Choudhary, K., Wines, D., Li, K., Garrity, K. F., Gupta, V., Romero, A. H., Krogel, J. T., Saritas, K., **Fuhr, A.**, Ganesh, P., Kent, P., Yan, K., Lin, Y., Ji, S., Blaiszik, B., Reiser, P., Friederich, P., Agrawal, A., Tiwary, P., Beyerle, E., Minch, P., Rhone, T. D., Takeuchi, I., Wexler, R. B., Mannodi-Kanakithodi, A., Ertekin, E., Mishra, A., Mathew, N., Baird, S. G., Wood, M., Rohskopf, A. D., Hattrick-Simpers, J., Wang, S-H., Achenie, L., Xin, H., Williams, M., Biacchi, A. J., Tavazza, F. Large Scale Benchmark of Materials Design Methods, *npj Comp. Mater.*, **2024** (Accepted)
 2. **Fuhr, A.**, Ganesh, P., Vasudevan, R. K., Roccapiore, K. M., Sumpter, B. G. Digital Twins and Deep Learning Segmentation of Defects in Monolayer MX₂ Phases, *Appl. Phys. Letters*, **2024**, 124, 3
 3. **Fuhr, A.**, Shields, A. E., Nykwest, E., Brubaker, Z. E., Niedziela, J. L., Miskowicz, A. J. Pressure modulated charge transfer and phonon interactions drive phase transitions in uranium–aluminum laves phases, *Comp. Mater. Sci.*, **2024**, 231, 112610
 4. Checa, M., **Fuhr, A.**, Sun, C., Vasudevan, R., Ziatdinov, Z., Ivanov, I., Yun, S-J., Xiao, K., Sehirlioglu, A., Kim, Y., Sharma, P., Kelley, K. P., Domingo, N., Jesse, S., Collins, L. High-speed mapping of surface charge dynamics using sparse scanning Kelvin probe force microscopy, *Nature Communications*, **2023**, 14, 71966
 5. **Fuhr, A.**, Sumpter, B. G., Ganesh, P. Defects go green: using defects in nanomaterials for renewable energy and environmental sustainability, *Front. Nano.*, 5, 1291338
 6. **Fuhr, A.**, Sumpter, B. G. Deep Generative Models for Materials Discovery and Machine Learning-Accelerated Innovation, *Front. Mater.*, **2022**, 9, 865270
 7. **Fuhr, A.**; Alexandrova, A. N.; Sautet, P. Stoichiometry-Controllable Optical Defects in Cu_xIn_{2-x}S_y Quantum Dots for Energy Harvesting, *J. Mater. Chem. A*, **2020**, 8, 12556-12565
 8. Du, J.; Singh, R.; Fedin, I.; **Fuhr, A.**; Klimov, V. I.; Spectroscopic Insights into High Defect Tolerance of Zn:CuInSe₂ Quantum-Dot-Sensitized Solar Cells, *Nature Energy*, **2020**, 5, 409417 (Cover Article)

9. **Fuhr, A.**; Yun, H. J.; Crooker, S. A.; Klimov, V. I. Spectroscopic and Magneto-Optical Signatures of Cu¹⁺ and Cu²⁺ Defects in Copper Indium Sulfide Quantum Dots, *ACS Nano*, **2020**, 14, 2212-2223
10. **Fuhr, A.**; Alexandrova, A. N.; Sautet, P. Heterogeneity in Local Chemical Bonding Explains Spectral Broadening in Quantum Dots with Cu Impurities, *J. Phys. Chem. C*, **2019**, 123, 5705-5713
11. Yun, H. J.; Lim, J.; **Fuhr, A.**; Keene, S.; Law, M.; Pietryga, J. M.; Klimov, V. I. Charge Transport Mechanisms in CuInSe_xS_{2-x} Quantum Dot Films, *ACS Nano*, **2018**, 12, 1258712596
12. **Fuhr, A.**; Yun, H. J.; Makarov, N. S.; Li, H.; McDaniel, H.; Klimov, V. I. Light Emission Mechanisms in CuInS₂ Quantum Dots Evaluated by Spectral Electrochemistry, *ACS Photonics*, **2017**, 4, 2425-2435
13. Cao, Y.; Li, X.; Bian, Z.; **Fuhr, A.**; Zhang, D.; Zhu, J.; Highly Photocatalytic Activity of Brookite/Rutile TiO₂ Nanocrystals with Semi-Embedded Structure, *Appl. Cat. B*. **2016**, 180, 551-553
14. Zheng, S-T; Zhao, X.; Lau, S.; **Fuhr, A.**; Feng, P.; Bu, X. Entrapment of Metal Clusters in MOF Channels by Extended Hooks Anchored at Open Metal Sites, *J. Am. Chem. Soc.* **2013**, 135, 10270-10273
15. Zheng, S.; Wu, T.; Chou, C-T; **Fuhr, A.**; Feng, P.; Bu, X. Development of Composite Inorganic Building Blocks for Metal-Organic Frameworks, *J. Am. Chem. Soc.* **2012**, 134, 4517-4520