

## Education

- **The Pennsylvania State University**  
*Ph.D. Materials Science and Engineering*  
– 4.0 GPA

**University Park, PA**  
2020 – 2024
  - **Beihang University (Beijing University of Aeronautics & Astronautics)**  
*B.S. Materials Science and Engineering; Minor, Mathematics*  
– 3.76 GPA  
– Merit Student (Top 4%)

**Beijing, China**  
2015 – 2019
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## Research Experience

- **Phases Research Lab, The Pennsylvania State University**  
*Graduate Research Assistant (Advisor: Prof. Zi-Kui Liu)*  
– First to apply thermodynamic modeling in the investigation of site nuclearity on Pd-Zn-based catalysts surfaces  
– Developed the Pd-Zn-based alloy thermodynamic databases and quantified uncertainty by leveraging the distribution of model parameters during optimization for accurate nuclearity design  
– Built framework to drive selections for stable intermetallic catalysts candidates with Machine Learning and first-principles calculations tools  
– Developed DFTTK structure builders to automatically generate structures for high-throughput computations

**University Park, PA**  
2020 – Present
  - **The Nuclear Science and Engineering Division, Argonne National Laboratory**  
*Research Aide Technical PhD (Advisor: Dr. Shayan Shahbazi)*  
– Developed LiF-LnF<sub>3</sub> thermodynamic databases to predict relative volatility of Ln  
– Quantified uncertainty and sensitivity of thermodynamic modeling of fluoride molten salts

**Lemont, IL**  
07/2022 – 09/2022
  - **International Research Institute for Multidisciplinary Science, Beihang University**  
*Undergraduate Research Assistant (Advisor: Prof. Qianfan Zhang)*  
– Built stable substrates with transition metal adsorbed on two-dimensional materials as catalysts  
– Designed performance analysis via computational methods to examine the thermodynamics and kinetics of hydrogen evolution reaction on the catalytic substrates

**Beijing, China**  
2017 – 2019
  - **Department of Materials Science and Engineering, Rensselaer Polytechnic Institute**  
*Undergraduate Research Assistant (Advisor: Prof. Yunfeng Shi)*  
– Investigated the corrosion process of the glass nanowire by using Molecular Dynamics simulations  
– Quantified the corrosion rate and analyzed the relationship between pre-tension and corrosion

**Troy, NY**  
2018
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## Teaching Experience

- **Department of Materials Science and Engineering, Penn State University**  
*Teaching Assistant*  
– MatSE 410: Phase Relations in Materials Systems

**University Park, PA**  
2021
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## Technical Skills

**Computational Tools and Software:** Python, MongoDB, VASP, Thermo-Calc, Matlab, ATAT  
**Software Developing:** DFTTK ([github.com/phasesresearchlab/dfttk](https://github.com/phasesresearchlab/dfttk))

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## Publications

3. A. Dasgupta, H. He, **R. Gong**, S. L. Shang, E. K. Zimmerer, R. J. Meyer, Z. K. Liu, M. J. Janik, and R. M. Rioux, Atomic Control of Active Site Ensembles in Ordered Alloys to Enhance Hydrogenation Selectivity, **Nature Chemistry**, 14, 523–529 (2022), [doi: 10.1038/s41557-021-00855-3](https://doi.org/10.1038/s41557-021-00855-3).
2. **R. Gong**, S. L. Shang, H. Sun, M. J. Janik, and Z. K. Liu, Thermodynamic modeling of the Pd-Zn system with uncertainty quantification and its implication to tailor catalysts, **Calphad**, 2022, [doi.org/10.1016/j.calphad.2022.102491](https://doi.org/10.1016/j.calphad.2022.102491).
1. J. P. S. Palma, **R. Gong**, B. J. Bocklund, R. Otis, M. Poschmann, M. Piro, Y. Wang, T. G. Levitskaia, S. Hu, H. Kim, S. L. Shang, and Z. K. Liu, Thermodynamic modeling with uncertainty quantification using the modified quasichemical model in quadruplet approximation: Implementation into PyCalphad and ESPEI, [arxiv.org/abs/2204.09111](https://arxiv.org/abs/2204.09111).