Rushi Gong

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Education

- **The Pennsylvania State University** — **University Park, PA**
  Ph.D. Materials Science and Engineering — *2020 – Present*
  - 4.0 GPA
- **Beihang University (Beijing University of Aeronautics & Astronautics)** — **Beijing, China**
  B.S. Materials Science and Engineering; Minor, Mathematics — *2015 – 2019*
  - 3.76 GPA
  - Merit Student (Top 4%)

Research Experience

- **Phases Research Lab, The Pennsylvania State University** — **University Park, PA**
  Graduate Research Assistant (*Advisor: Prof. Zi-Kui Liu*) — *2020 – Present*
  - 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
  - Projects:
    - DOE-BES: Data-driven discovery of intermetallic catalysts with controlled active site nuclearity
    - DOE-NEUP: High throughput computational platform for predictive modeling of thermochemical and thermophysical properties of fluoride molten salts
- **International Research Institute for Multidisciplinary Science , Beihang University** — **Beijing, China**
  Undergraduate Research Assistant (*Advisor: Prof. Qianfan Zhang*) — *2017 – 2019*
  - 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
- **Department of Materials Science and Engineering, Rensselaer Polytechnic Institute** — **Troy, NY**
  Undergraduate Research Assistant (*Advisor: Prof. Yunfeng Shi*) — *2018*
  - Investigated the corrosion process of the glass nanowire by using Molecular Dynamics simulations
  - Quantified the corrosion rate and analyzied the relationship between pre-tension and corrosion

Teaching Experience

- **Department of Materials Science and Engineering, Penn State University** — **University Park, PA**
  Teaching Assistant — *2021*
  - MatSE 410: Phase Relations in Materials Systems

Technical Skills

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

Publications

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**, 2022, doi: 10.1038/s41557-021-00855-3.

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, submitted, arxiv.org/abs/2203.00044.

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.