Rushi Gong

(814) 441-2268 • rsgong@psu.edu

Education

- **The Pennsylvania State University** — **University Park, PA**
  Ph.D. Materials Science and Engineering — *2020 – 2024*
  - 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*
  - Developed the Pd-Zn-based alloy thermodynamic databases and quantified uncertainty for accurate nuclearity design in catalysts
  - First to apply Bayesian statistics and model selection for selecting liquid solution models in CALPHAD modeling
  - Improved functionalities of computational thermodynamics tools PyCalphad and ESPEI for molten salts properties prediction
  - Developed DFTTK structure builders to automatically generate structures for high-throughput computations
- **The Nuclear Science and Engineering Division, Argonne National Laboratory** — **Lemont, IL**
  Research Aide Technical PhD (*Advisor: Dr. Shayan Shahbazi*) — *07/2022 – 09/2022, 05/2023 – 08/2023*
  - Developed and quantified uncertainty of LiF-LnF3 thermodynamic databases to predict vapor-liquid equilibrium properties for distillation system design in Molten Salt Reactor
  - Developed frameworks for calculating the Ellingham diagram to quantify redox potential of metals in fluoride molten salts
- **International Research Institute for Multidisciplinary Science, Beihang University** — **Beijing, China**
  Undergraduate Research Assistant (*Advisor: Prof. Qianfan Zhang*) — *2017 – 2019*
  - Designed performance analysis via computational methods to examine the thermodynamics and kinetics of hydrogen evolution reaction on the transition metal adsorbed on two-dimensional 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 analyzed the relationship between pre-tension and corrosion

Technical Skills

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

Teaching Experience

- **Department of Materials Science and Engineering, Penn State University** — **University Park, PA**
  Teaching Assistant — *2021 – Present*
  - (*Fall 2023*) MatSE 580: Computational Thermodynamics
  - (*Fall 2022*) MatSE 581: Computational Kinetics
  - (*Spring 2021, Spring 2023*) MatSE 410: Phase Relations in Materials Systems

Awards

- MATSE Travel Award for MS&T 23 Conference, Pennsylvania State University — *2023*
- NSF Scholarship, Calphad L Conference — *2023*
- Thrower Travel Award for Calphad L Conference, Pennsylvania State University — *2023*

Publications

4. J.P.S. Palma, **R. Gong**, B.J. Bocklund, R. Otis, M. Poschmann, M. Piro, Y. Wang, S. Shahbazi, T.G. Levitskaia, S. Hu, N.D. Smith, H. Kim, Z.K. Liu, and S.L. Shang, Thermodynamic modeling with uncertainty quantification using the modified quasichemical model in quadruplet approximation: Implementation into PyCalphad and ESPEI, arxiv.org/abs/2204.09111.

3. H. Sun, S.L. Shang, **R. Gong**, B.J. Bocklund, A.M. Beese, Z.K. Liu, Thermodynamic modeling of the Nb-Ni system with uncertainty quantification using PyCalphad and ESPEI, **Calphad**, 2023, doi.org/10.1016/j.calphad.2023.102563.

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.

1. 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.

Presentations

3. **R. Gong***, S.L. Shang, V. Goncharov, B. Merrill, X. Guo, Z.K. Liu (2023, October) *Invited*. Exploring and Implementing Thermodynamic Models for Liquid and their Applications to Thermodynamic Modeling of Molten Salts. Materials Science and Technology 2023, Columbus, OH.

2. **R. Gong***, S. Shahbazi (2023, July). Thermodynamic Modeling and Model Selection for LiF-LnF3 Molten Salts with Uncertainty Propagation. Molten Salt Thermal Properties Uncertainty Workshop, Lemont, IL.

1. **R. Gong***, S.L. Shang, G. Canning, R.M. Rioux, M.J. Janik, Z.K. Liu (2022, October). Thermodynamic Modeling with Uncertainty Quantification and its Implications for Intermetallic Catalysts Design: Application to PdZn-Based Gamma-Brass Phase. Materials Science and Technology 2022, Pittsburgh, PA.

***** *presenter*