Rushi Gong

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Education

- **The Pennsylvania State University** — **University Park, PA**
  Ph.D. in Materials Science and Engineering — *2020 – Present*
  - GPA: 4.0/4.0
- **Beihang University** — **Beijing, China**
  B.S. in Materials Science and Engineering; Minor, Mathematics — *2015 – 2019*
  - GPA: 3.76/4.0, 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 Pd-Zn-based gamma-brass alloys using DFT-based first-principles calculations, machine learning, and CALPHAD modeling with uncertainty quantification and propagation to achieve atomic control of catalytic active-site ensembles and enhance the hydrogenation selectivity of catalysts.
  - Developed thermodynamic databases with uncertainty quantification using CALPHAD modeling, DFT calculations, and AIMD simulations for molten salts, including Cr and Ni in FLiNaK and LaCl3 in LiCl-KCl, improved the accuracy of predicting phase stability and other thermodynamic properties of molten salts solids and liquids.
  - Applied Bayesian methodologies and Bayesian model selections in CALPHAD modeling, achieved the statistical comparison of different liquid solution models, including ionic model and modified quasichemical model, effectively optimized models through the Markov Chain Monte Carlo method, quantified uncertainty to enhance the accuracy and reliability of thermodynamic models.
  - Designed a framework and template creator for integrating thermodynamic models with the CALPHAD method and implementing custom models into the open-source software PyCalphad. Led the implementation of the universal quasichemical model and molecular interaction volume model, expanding their accessibility and usability across multiple disciplines.
  - Established the structure builder in the open-source software DFTTK to automatically generate structures for high-throughput DFT calculations and CALPHAD modeling.
- **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 performed uncertainty quantification and propagation of LiF-LnF3 thermodynamic databases to facilitate accurate predictions of vapor-liquid equilibrium properties for designing distillation systems in Molten Salt Reactors.
  - Enhanced and upgraded functionalities of open-source computational thermodynamics software PyCalphad and ESPEI to predict thermodynamic properties of molten salts. Implemented features including the Ellingham diagram calculations, redox potential calculations for corrosion properties, vapor pressure calculations, and improved calculation stability on multi-component systems.
- **International Research Institute for Multidisciplinary Science, Beihang University** — **Beijing, China**
  Undergraduate Research Assistant (*Advisor: Prof. Qianfan Zhang*) — *2017 – 2019*
  - Investigated electronic structure of two-dimensional material FeOCl through DFT calculations, applied strain and doping to control magnetic properties.
  - Developed a performance analysis framework using DFT calculations to investigate the thermodynamics and kinetics of the hydrogen evolution reaction on transition metals 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 approaches: CALPHAD, DFT, Ab initio Molecular Dynamics (AIMD), Machine learning
Computational languages and tools: Python, Linux, Matlab, GitHub, VASP, Thermo-Calc, ATAT, MongoDB, LAMMPS
Software developing: PyCalphad, ESPEI, and DFTTK. (github.com/RushiGong)

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 Awards, Pennsylvania State University — *2023, 2024*
- NSF Scholarship, Calphad L Conference — *2023*
- Thrower Travel Award for Calphad L Conference, Pennsylvania State University — *2023*

Publications

7. **R. Gong**, S.L. Shang, Y. Wang, J.P.S. Palma, H. Kim, and Z.K. Liu, Revisiting thermodynamics in (LiF, NaF, KF, CrF2)-CrF3 by first-principles calculations and CALPHAD modeling, **submitted**, 2024, doi: arXiv:2402.12574.
6. S.L. Shang, **R. Gong**, M.C. Gao, D. Pagan, and Z.K. Liu, Revisiting First-Principles Thermodynamics by Quasiharmonic Approach: Application to Study Thermal Expansion of Additively-Manufactured Inconel 625, **submitted**, 2024, doi: 10.2139/ssrn.4763242.
5. S. Shahbazi, M. Tano, S. Thomas, S. Walker, A.A. Jaoude, Y. Jeong, **R. Gong**, D.H. Kam, B. Chen, D. Grabaskas, NEAMS activities supporting mechanistic source term model development for molten salt reactors, **PSA conference**, 2023, doi: 10.13182/PSA23-41261.
4. J.P.S. Palma, **R. Gong**, B.J. Bocklund, R. Otis, M. Poschmann, M. Piro, S. Shahbazi, T.G. Levitskaia, S. Hu, N.D. Smith, Y. Wang, 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, **Calphad**, 83, (2023), doi: 10.1016/j.calphad.2023.102618.
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**, 82, (2023), doi: 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**, 79, (2022), doi: 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

4. **R. Gong***, S.L. Shang, V. Goncharov, B. Merrill, X. Guo, Z.K. Liu (2024, March). Uncertainty Quantification and Sensitivity Analysis of Advanced Models for Thermodynamic Modeling of Molten Salt System. TMS Annual Meeting and Exhibition 2024, Orlando, FL.
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*