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*
  - Applied Bayesian inference and uncertainty quantification in CALPHAD (CALculation of PHAse Diagram) modeling through the Markov Chain Monte Carlo (MCMC), first achieved Bayesian model selection for multi-component mixture solution models, enhancing modeling efficiency and reliability.
  - Data-driven development of Pd-Zn-based gamma-brass alloys through computational thermodynamics and machine learning neural networks, achieved atomic control of catalytic active-site ensembles and increased ethylene hydrogenation activity by 100%.
  - Investigated atomic environments and energy of molten salts using ab initio molecular dynamics (AIMD), developed thermodynamic databases with uncertainty quantification and improved the accuracy of molten salts energy prediction by 20%. Molten salts involved: structural materials Cr and Ni and fission products La in fluoride and chloride molten salts.
  - Designed a template generator for implementing thermodynamic models into PyCalphad for high-throughput modeling with uncertainty quantification. Thermodynamic models involved: the universal quasichemical model, molecular interaction volume model, and Peng-Robinson equation of state.
  - Established the structure builder in DFTTK for automating structure generation and integrated it into an automatic workflow 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 LiF-LnF3 thermodynamic databases with uncertainty quantification and propagation, accurately predicted vapor-liquid equilibrium properties for designing distillation systems in Molten Salt Reactors.
  - Enhanced and upgraded functionalities of PyCalphad and ESPEI for molten salts thermodynamic properties calculations. 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 through Nudged Elastic Band (NEB).
- **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, AIMD, Machine learning
Computational languages and tools: Python, Linux, Matlab, GitHub, VASP, Thermo-Calc, MongoDB, JSON, 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. 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, **Scripta Materialia,** 250 (2024) 116200. doi: 10.1016/j.scriptamat.2024.116200.

6. **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, **Calphad**, 85, (2024), doi: 10.1016/j.calphad.2024.102703.

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*