Ruiyu Wang

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Education

Ph.D. in Chemistry, Temple University 2022
Advisors: Prof. Eric Borguet, Prof. Vincenzo Carnevale

M.Sc. in Chemistry, Nankai University 2016
Advisor: Prof. Tianying Guo

B.Sc. in Chemistry, Nankai University 2013

Work Experience

Postdoc researcher, University of Maryland, College Park 2022 - Present
Advisor: Prof. Pratyush Tiwary

Research Interests

Molecular Dynamics (MD) Simulations, Machine Learning based Enhanced Sampling, Water Interfaces, Catalytic materials, Generative AI, Nucleation

Publications (Google Scholar)

("#" represents equal contributions)

Publications in Preparation:

20. **Wang, R.#**, Lee, S.#, Debenedetti, P., Tiwary P., Inferring water liquid-liquid phase transition using generative AI from limited data. *in preparation*.
19. **Wang, R.#**, Meraz V.#, Tiwary P., Machine Learning Driven Advances in Molecular Dynamics of Solvated, Interfacial Systems. ***Chem. Soc. Rev.*** *in review*. (preprint)
18. Lee, S.#, **Wang, R.#**, Herron, L., Tiwary P., Exponentially Tilted Thermodynamic Maps (expTM): Predicting Phase Transitions Across Temperature, Pressure, and Chemical Potential. ***Nat. Comm.*** *in revision*. (preprint)

Five Selected Publications:

17. **Wang, R.**, Tiwary P., Electric Field's Dueling Effects through Dehydration and Ion Separation in Driving NaCl Nucleation at Charged Nanoconfined Interfaces. ***J. Am. Chem. Soc.*** **2025**, *147*, 16876-16884. (PDF, preprint)
16. **Wang, R.**, Remsing, R. C., Klein, M. L., Borguet, E. & Carnevale, V., On the Role of α-alumina in the Origin of Life: Surface Driven Assembly of Amino Acids. ***Sci. Adv.*** **2025**, *11*, eadt4151. (PDF)
15. **Wang, R.**, Tiwary P., Enhanced Polymorph Metastability Drives Glycine Nucleation in Aqueous Salt Solutions. ***Proc. Natl. Acad. Sci. U.S.A.*** **2025**, *122*, e2503490122. (PDF)
14. **Wang, R.**, Tiwary, P., Atomic scale insights into NaCl nucleation in nanoconfined environments. ***Chem. Sci.*** **2024**, 15391-15398. (PDF)
13. Xu, P.#, **Wang, R.#**, Zhang, H., Carnevale, V., Borguet, E., Suntivich, J., Cation Modifies Interfacial Water Structures on Platinum during Alkaline Hydrogen Electrocatalysis. ***J. Am. Chem. Soc.*** **2024,** 146, 4, 2426-2434. (PDF)

Other Papers:

12. Tiwary, P., Herron, L.#, John, R.#, Lee, S.#, Sanwal D.# & **Wang, R.#**, Generative Artificial Intelligence for Computational Chemistry: a Roadmap to Predicting Emergent Phenomena. ***Proc. Natl. Acad. Sci. U.S.A.*** **2025**, accepted. (preprint)
11. **Wang, R.**, DelloStritto, M., Klein, M. L., Borguet, E., Carnevale, V., Topological Properties of Interfacial Hydrogen Bond Networks. *Phys. Rev. B* **2024**, *110*, 014105. (PDF, preprint)
10. **Wang, R.**, Mehdi S., Zou, Z., Tiwary P., Is the Local Ion Density Sufficient to Drive NaCl Nucleation in Vacuum and in Water? *J. Phys. Chem. B* **2024**, 128, 4, 1012–1021. (PDF, preprint)
9. **Wang, R.**, Remsing, R. C., Klein M., Carnevale V. & Borguet E., Superhydrophilicity of α-Alumina Surfaces Results from Tight Binding of Interfacial Waters to Specific Aluminols. *J. Colloid Interface Sci.* **2022**, 628, 943-954. (PDF, preprint)
8. **Wang, R.**, Klein M., Carnevale V. & Borguet E., Investigation of Water/solid Interfaces by Molecular Dynamic Simulations. ***Wiley Interdiscip. Rev. Comput. Mol. Sci.*** **2021**, e1537. (PDF)
7. **Wang, R.**, Carnevale V., Klein M. & Borguet E. First Principles Calculation of Water pKa Using the Newly Developed SCAN Functional. *J. Phys. Chem. Lett.* **2020**, *11*, 54-59. (PDF)
6. **Wang, R.**, DelloStritto, M., Remsing, R. C., Carnevale, V., Klein, M. L. & Borguet, E., Sodium Halide Adsorption and Water Structure at the α-Alumina(0001)/Water Interface. *J. Phys. Chem. C* **2019**, *123*, 15618-15628. (PDF)
5. **Wang, R.**, Pan, J., Qin, M., & Guo, T., Molecularly Imprinted Nanocapsule Mimicking Phosphotriesterase for the Catalytic Hydrolysis of Organophosphorus Pesticides. *Eur. Polym. J* **2019**, *110*, 1-8. (PDF)
4. Shi, H., **Wang, R.**, Yang, J., Ren, H., Liu, S., & Guo, T., Novel Imprinted Nanocapsule with Highly Enhanced Hydrolytic Activity for Organophosphorus Pesticide Degradation and Elimination. *Eur. Polym. J* **2015**, *72*, 190-201. (PDF)
3. Liu, Z., Liu, S., Shi, H., Ren, H., **Wang, R.**, Yang, J., & Guo, T., Fluorescently Labeled Degradable Thermoplastic Polyurethane Elastomers: Visual Evaluation for the Degradation Behavior. *J. Appl. Polym. Sci* **2015**, *132*(36).
2. Chi, W., Liu, S., Yang, J., **Wang, R.**, Ren, H., Zhou, H., Chen, J. & Guo, T., Evaluation of the Effects of Amphiphilic Oligomers in PEI Based Ternary Complexes on the Improvement of pDNA Delivery. *J. Mater. Chem. B* **2014**, *2*(33), 5387-5396.
1. Guo, Y., **Wang, R.**, Chi, W., Liu, S., Shi, H., & Guo, T., One-step Synthesis of Reactant-Product-dual-template Imprinted Capsules as Phosphotriesterase Mimetic Enzymes for Pesticide Elimination. *RSC Adv* **2014**, *4*(16), 7881-7884. (PDF)

Grants

(active) PI. ACCESS program, Topological properties of hydrogen bond networks of ion solutions near charged electrode surfaces, CHE250110, 2025-2026 (200k CPU hours).

Research Experience:

- **Prediction of phase diagram using generative AI.** (2024-present)
  - Developed structural descriptors for Lennard-Jones particles, CO_2, and water for training generative AI models to infer phase behavior.
- **Investigation of phase transition various environments using machine learning-assisted enhanced sampling molecular dynamics simulations.** (2019-2025)

  - Designed and implemented MD simulations with enhanced sampling to study the nucleation of NaCl from aqueous solutions in bulk liquid and under nanoconfinement. Estimated and analyzed nucleation mechanisms with ML models.
  - Designed, implemented, and analyzed MD simulations of glycine aggregation at alumina interfaces with enhanced sampling.
- **Investigation of water wetting and ion adsorption at water/solid interfaces.** (2016-2022)
  - Developed in-house Python tools to analyze structure and dynamics of interfacial water.
  - Calculated nonlinear optical response to interpret experimental measurements.
  - Developed a graph model to quantify the high connectivity of interfacial hydrogen bond networks.
- **Calculation of bulk water pKa using DFT-MD.** (2018)
  - Conducted DFT-MD simulations and modified the Quantum Espresso code for free energy calculations.

Skills

GROMACS, VASP, Quantum-Espresso, Gaussian 09, CP2k, ChemOffice
C++, Python (Numpy, sklearn, Keras, Pytorch), C, Linux

Awards

- Doctoral Dissertation Completion grant. Temple University, 2022
- College of Science and Technology Outstanding Research Assistant (RA) Award. (1 winner from all PhD students in the department) Temple University, 2021
- The Daniel Swern Research Award. Temple University, 2021
- Student Travel Awards: GEOC ACS Spring 2020 Philadelphia. ACS, 2019
- Presidential Fellowship. Temple University, 2016
- TEDA-Asymchem Scholarship. Nankai University, 2014
- The Third Prize of Excellent Undergraduate Scholarship in the academic year of 2011-2012. Nankai University, 2012
- The Second Prize of Excellent Undergraduate Scholarship in the academic year of 2010-2011. Nankai University, 2011
- The Second Prize of Excellent Undergraduate Scholarship in the academic year of 2009-2010. Nankai University, 2010

Presentations

- Investigation of nucleation and assembly at nanoscaled aqueous interfaces using AI augmented enhanced sampling
  - Postdoctoral Research Symposium, University of Maryland 2024
  - Gordon Research Seminar (**discussion leader**) & Gordon Research Conference 2024
- On the Role of α-Alumina in the Origin of Life: Surface Driven Assembly of Amino Acids
  - ACS (spring) National Meeting (**ACS student travel award winner**) 2021
- Water hydrophilic behavior at aqueous/alumina interfaces
  - ACS (spring) National Meeting 2021
  - ACS YCC Poster Session, Philadelphia 2020

- Ion Solutions at Mineral/Water Interfaces: Bridging the Gap between Computational Modeling and Spectroscopy
  - ICCAS Beijing, China 2019
  - ICMS, Temple University 2019
- First Principles Calculation of Water pKa Using the Newly Developed SCAN Functional
  - SCAN Workshop, Temple University 2019
  - Penn Conference in Theoretical Chemistry, University of Pennsylvania 2019
- Investigation of the charged Al2O3(0001) surface in acidic and basic solutions by ab initio MD simulations
  - Penn Conference in Theoretical Chemistry, University of Pennsylvania 2018
- Ion adsorption and water dynamics near α-alumina (0001)/water interface
  - ACS YCC Poster Session, Philadelphia 2018
- Ion adsorption and water behavior near α-alumina (0001)/water interface
  - ACS National Meeting, Washington, D.C. 2017
  - Penn Conference in Theoretical Chemistry, University of Pennsylvania 2017
- Adsorption of Sodium Halides to the Water-Air and Water-Alumina Interfaces
  - ACS YCC Poster Session, Philadelphia 2017
  - Water Workshop, Temple University 2017

Professional Affiliations

Member of American Chemical Society, the Electrochemical Society, American Physical Society, Python Software Foundation

Mentoring

Kevin Millan. Intern student at Temple University, 2017.
Dorian Louaas. Intern student at Temple University, 2020.
Jordan Wenning. Undergraduate student at Temple University, 2021.
Richard John. PhD student at University of Maryland, 2024-2025.

Service

Reviewing Proc. Natl. Acad. Sci. U.S.A, npj Comput. Mater., J. Chem. Theory Comput, J. Chem. Phys, and J. Phys. Chem.