Ruiyu Wang

Email: rywang@umd.edu, ruiyuwang_work@outlook.com

Education

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

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

Research interests

- Molecular Dynamics Simulations
- Machine Learning based Enhanced Sampling
- Water, Interfaces, and materials
- Generative AI
- Nucleation

Research experience:

- **Investigation of nucleation of NaCl at various environments using machine learning-assisted enhanced sampling molecular dynamics simulations** (U. of Maryland, 2022-2025)
  I designed enhanced sampling molecular dynamics (MD) simulations to study the phase transition of NaCl aqueous solutions. By utilizing high-dimensional simulation data with appropriate machine learning, I quantified the role of solutes during nucleation processes, which is often overlooked before. Additionally, I designed simulations to reveal how nanoconfined materials promote nucleation.
- **Predicting phase diagram using generative AI** (U. of Maryland, 2024-present)
  I developed structural descriptors for Lennard-Jones particles and trained a generative AI model capable of predicting a complete phase diagram using just two data points. The AI model successfully reproduces the behavior of Lennard-Jones particles. Currently, I am tuning the model to extend its capabilities to more complex molecules.
- **Biomolecule adsorption and the origin of lives** (Temple University, 2019-2023)
  I designed enhanced sampling MD simulations to investigate the aggregation of glycine, which is extremely rare in bulk water. My simulations demonstrate that the adsorption, self-assembly, and dissolution of amino acids at water/oxide interfaces drives the enrichment of biomolecules, a critical step in the abiogenesis process.
- **Water wetting and ion adsorption at water/solid interfaces** (Temple University, 2016-2022)
  I developed in-house Python code to analyze the structure and dynamics of interfacial water. I calculated the nonlinear optical response, which matches experimental measurements and

received highly positive feedback from reviewers of *JACS*. Additionally, I developed a graph model to measure the universal high connectivity of interfacial hydrogen bond networks quantitatively.

- **Calculation of bulk water pKa using DFT-MD** (Temple University, 2018)
  I conducted DFT-MD simulations and modified the Quantum Espresso code to collect forces during constraint-MD, enabling the calculation of the free energy surface for the self-ionization of bulk water.

Publications (Google Scholar)

"#" represents equal contributions. Five selected are highlighted.

19. Lee, S.#, **Wang, R.#**, Herron, L., Tiwary P., Predicting Chemical Properties at Environments outside Training Data with Generative AI & Statistical Mechanics. *submitted*. (preprint)
18. **Wang, R.**, Meraz V., Tiwary P., Machine Learning Driven Advances in Molecular Dynamics of Solvated, Interfacial Systems. *Chem. Soc. Rev (invited)*. *Under preparation*.
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**, *(in revision).* (preprint)
16. **Wang, R.**, Tiwary P., Enhanced Polymorph Metastability Drives Glycine Nucleation in Aqueous Salt Solutions. **2025**, *Proc. Natl. Acad. Sci. U.S.A. (accepted).*
15. Tiwary, P., Herron, L.#, John, R.#, Lee, S.#, Sanwal D.# & **Wang, R.#**, Generative Artificial Intelligence for Computational Chemistry: a Roadmap to Predicting Emergent Phenomena. **2025**, *Proc. Natl. Acad. Sci. U.S.A. (accepted).* (preprint)
14. **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. **2025**, *Sci. Adv*. *(accepted).* (preprint)
13. **Wang, R.**, Tiwary P., Atomic Scale Insights into NaCl Nucleation in Nanoconfined Environments. *Chem. Sci.* **2024**. DOI: 10.1039/D4SC04042B. (PDF)
12. **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)
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. 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, 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, preprint)

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, preprint)
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, preprint)
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)

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

Skills

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

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, J. Chem. Theory Comput, J. Chem. Phys, and J. Phys. Chem.

References

Prof. Vincenzo Carnevale, & Prof. Eric Borguet

Note: Both Prof. Carnevale and Prof. Borguet are my PhD advisors. They will submit one joint co-signed recommendation letter, uploaded by Prof. Carnevale.
Institute for Computational Molecular Science (V.C.), Department of Chemistry (E.B.), Temple University
Phone: 2152044214 (V.C.), 2152049696 (E.B.)
Website: https://carnevalelab.org/index.html (V.C.), https://sites.temple.edu/borguet/eric-borguet/ (E.B.)
Email: vincenzo.carnevale@temple.edu (V.C.), eborguet@temple.edu (E.B.)

Prof. Michael L. Klein

Institute for Computational Molecular Science, Temple University
Phone: 2152044212
Website: https://icmshpc.com/team/
Email: mlklein@temple.edu

Prof. Pratyush Tiwary

Institute for Physical Science and Technology, University of Maryland, College Park
Phone: 3014052148
Website: https://sites.google.com/site/pratyushtiwary/group?authuser=0
Email: ptiwary@umd.edu