

# 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, 2022-2024)  
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. (Two first-author papers published)
- **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 life** (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. (One first-author paper under review)
- **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. (Five first-author papers published)

- **Calculation of bulk water pKa using the SCAN functional** (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. (One first-author paper published)

## Publications ([Google Scholar](#))

“#” represents equal contributions. Five papers are highlighted.

18. Lee, S.#, **Wang, R.#**, Herron, L., Tiwary P., Predicting Chemical Properties at Environments outside Training Data with Generative AI & Statistical Mechanics. *Under preparation*.
17. **Wang, R.**, Meraz V., Tiwary P., Machine Learning Driven Advances in Molecular Dynamics of Solvated, Interfacial Systems. *Chem. Soc. Rev (invited) 2024. Under preparation*.
16. **Wang, R.**, Tiwary P., Electric Field's Dueling Effects through Dehydration and Ion Separation in Driving NaCl Nucleation at Charged Nanoconfined Interfaces. **2024. JACS (under review).** ([preprint](#))
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. **2024. 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  $\alpha$ -alumina in the Origin of Life: Surface Driven Assembly of Amino Acids. **2024. Sci. Adv. (under minor revision).** ([preprint](#))
13. **Wang, R.**, Tiwary P., Atomic Scale Insights into NaCl Nucleation in Nanoconfined Environments. *Chem. Sci.* **2024**. DOI: 10.1039/D4SC04042B. ([PDF](#), [preprint](#))
12. **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](#))
11. **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](#))
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  $\alpha$ -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  $\alpha$ -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  $\alpha$ -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  $\text{Al}_2\text{O}_3(0001)$  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  $\alpha$ -alumina (0001)/water interface
  - ACS YCC Poster Session, Philadelphia 2018
- Ion adsorption and water behavior near  $\alpha$ -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

## Service

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