

# 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

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

## Research Interests

Molecular Dynamics 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. Rev.* *in revision*. ([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  $\alpha$ -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**, *15*, 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:

# Ruiyu Wang

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**, 122, e2415655121. ([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. **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.**, Zou, Y.; Remsing, R. C.; Ross, N. O.; Klein, M. L.; 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](#))
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  $\alpha$ -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).

## Skills

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

## Awards

- Doctoral Dissertation Completion grant

Temple University, 2022

# Ruiyu Wang

- 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 (Water and Aqueous Solutions) 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 Al<sub>2</sub>O<sub>3</sub>(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

**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, npj Comput. Mater., J. Chem. Theory Comput., J. Chem. Phys., and J. Phys. Chem.