Ruiyu Wang

Contact

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Experience

University of Maryland, College Park, 2022 - 2023
Postdoc researcher. (Advisor: Prof. Pratyush Tiwary)

Education

Ph.D. in Chemistry, Temple University 2022
"Understanding aqueous solutions at α-alumina surfaces using molecular dynamics simulations" (Advisor: Dr. Eric Borguet, Dr. Vincenzo Carnevale)

M.Sc. in Chemistry, Nankai University 2016

B.Sc. in Chemistry, Nankai University 2013

Research interests

Molecular Dynamics Simulations
Machine Learning Enhanced Sampling
Water Interfaces
Vibrational Spectra Prediction
Nucleation

Skills

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

Selected Publications

*: I am (one of) corresponding author(s). #: Authors contribute equally.

At UMD

12. **Wang, R.**; Zou, Z.; Mehdi S.; and Tiwary P., Is the local ion density sufficient to drive NaCl nucleation in vacuum and in water? *Submitted*, **2023**. (preprint)

At Temple University

11. Xu, P.#; **Wang, R.#**; Zhang, H.; Carnevale, V.; Borguet, E.; Suntivich, J., Cation Modifies Interfacial Water Structures on Platinum during Alkaline Hydrogen Electrocatalysis. *Submitted*, **2023**. (preprint)
10. **Wang, R.**; DelloStritto, M.; Klein, M. L.; Borguet, E.; Carnevale, V., Topological properties of interfacial hydrogen bond networks. *Submitted*, **2023**.
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)

Other Publications

At Temple University

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)

At Nankai University

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
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

Awards

Doctoral Dissertation Completion grant. Temple University, 2021
College of Science and Technology(CST) Outstanding Research Assistant (RA) Award. Temple University, 2021
The Daniel Swern Research Award. Temple University, 2021
Student Travel Awards: GEOC ACS Spring 2020 Philadelphia. 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

1. “On the Role of α-Alumina in the Origin of Life: Surface Driven Assembly of Amino Acids” (ACS student travel award winner), ACS National Meeting Spring 2021
2. “Water hydrophilic behavior at aqueous/alumina interfaces”, ACS National Meeting Spring 2021
3. “Ion Solutions at Mineral/Water Interfaces: Bridging the Gap between Computational Modeling and Spectroscopy”, ICCAS Beijing, China, 2019; ICMS, Temple University, USA. 2019
4. “First Principles Calculation of Water pKa Using the Newly Developed SCAN Functional”, Workshop: FUNCTIONAL: FUNDAMENTALS, PRACTICES, AND EXTENSIONS, Temple University, 2019; Penn Conference in Theoretical Chemistry, University of Pennsylvania, 2019
5. “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

6. “Ion adsorption and water dynamics near α-alumina (0001)/water interface”, ACS YCC Poster Session and Grad School/Career Fair, Philadelphia. 2018
7. “Ion adsorption and water behavior near α-alumina (0001)/water interface”, ACS 254th National Meeting & Exposition, Washington, D.C. 2017; Penn Conference in Theoretical Chemistry, University of Pennsylvania, 2017
8. “Adsorption of Sodium Halides to the Water-Air and Water-Alumina Interfaces”, ACS YCC Poster Session and Grad School/Career Fair, Philadelphia. 2017; Experimental and Computational Approaches to Understanding Aqueous Interfaces workshop, Temple University, 2017

Professional Affiliations

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