Ruiyu Wang

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RESEARCH INTERESTS

Molecular Dynamics Simulations
Water/oxide Interfaces
Free Energy Calculation
Vibrational Spectra Prediction
Machine Learning

SKILLS

GROMACS, VASP, Quantum-Espresso, Gaussian 09, CP2k, Chemoffice
C++, Python (Numpy, Sklearn, Keras), C, Linux
Machine Learning

WORK EXPERIENCE

Post-doc. With Prof. Pratyush Tiwary, University of Maryland. 2022 - now

EDUCATION

Ph.D., Chemistry, Department of Chemistry, CST, Temple University. 2016 - 2022

- *Understanding Aqueous Solutions at α-Alumina Surfaces Using Molecular Dynamics Simulations.* Supervisor: Dr. Eric Borguet, Dr. Vincenzo Carnevale

M.Sc. in Chemistry, Institute of Polymer Chemistry, College of Chemistry, Nankai University. 2013 - 2016

- *Synthesis and Mechanism Study of Enzyme Imitation Molecular Imprinted Nanocapsule for Catalyzing Hydrolysis of Organophosphorus Pesticide.* Supervisor: Prof. Tianying Guo

B.Sc. in Chemistry, College of Chemistry, Nankai University. 2009 - 2013

- *Preparation of a Functional Polymersome.* Supervisor: Prof. Tianying Guo

SELECTED PUBLICATIONS

(At Temple University)

Wang, R.#; DelloStritto, M.#; Klein, M. L.; Borguet, E.; Carnevale, V., Increased Connectivity and Reduced Dimensionality of Hydrogen Bond Networks at Interfaces. *In preparation*, **2022**.

Wang, R., Zou, Y., Remsing, R. C., Ross, N. O., Klein, M. L., Borguet, E. & Carnevale, V., On the Role of α-alumina in the Origin of Life: Surface Driven Assembly of Amino Acids. *Submitted*, **2022**.

Wang, R.*; Zou, Y.; Remsing, R. C.; Ross, N. O.; Klein, M. L.; 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. (link, preprint)

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. (link)

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. (link)

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. (link)

(At Nankai University)

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. (link)

(#: contributed equally; *: corresponding author)

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

REFERENCES

Dr. Eric Borguet advisor eborguet@temple.edu
Professor, Department of Chemistry, Temple University

Dr. Vincenzo Carnevale advisor vincenzo.carnevale@temple.edu
Research Professor, Department of Biology, Temple University

Dr. Michael L. Klein co-author, dissertation committee mlklein@temple.edu
Dean, College of Science & Technology, Temple University
Member of US National Academy of Sciences

OTHER PUBLICATIONS

(At Nankai University)

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

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)

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

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

PRESENTATIONS

CONFERENCE

On the Role of α-Alumina in the Origin of Life: Surface Driven Assembly of Amino Acids (ACS student travel award winner)
Water hydrophilic behavior at aqueous/alumina interfaces
ACS National Meeting Spring 2021, online

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

Investigation of the charged Al_2O_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 α-alumina (0001)/water interface
ACS YCC Poster Session and Grad School/Career Fair, Philadelphia. 2018

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

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

SEMINAR

Ion Solutions at Mineral/Water Interfaces: Bridging the Gap between Computational Modeling and Spectroscopy.
ICCAS Beijing, China, 2019

ICMS, Temple University, USA. 2019

RESEARCH PROJECTS

(At Temple University)
Supervisor: Eric Borguet, Vincenzo Carnevale

Ion adsorptions at platinum/water interfaces and the applications in electrochemistry (2022-)
Other Collaborators: Pengtao Xu

The role of α-alumina(0001)/water interfaces for life origin (2019-)
Other Collaborators: Richard C. Remsing

Calculations of pKa by recently developed SCAN functional (2018-2019)
Other Collaborators: Richard C. Remsing, Mark DelloStritto

Dynamics, hydrogen bond structures and vibrational analysis at the neutral alumina/water interface (2018-2022)
Other Collaborators: Stefan Piontek, Richard C. Remsing, Mark DelloStritto, Tim Marshall, Yunqian Zou, Naomi Olivia Ross

Calculations of the vSFG of alumina (0001)/water interfaces in acidic or basic solutions by SCAN functional (2017-2020)
Other Collaborators: Mark DelloStritto

Ion adsorption near the alumina (0001)/water interface by molecular dynamics simulations (2016-2018)
Other Collaborators: Richard C. Remsing, Mark DelloStritto

(At Nankai University)
Supervisor: Tianying Guo

Mechanism study for molecular imprinted polymers as enzyme imitation using Density Function Theory method (2015-2016)
Co-advisor: Mingtao Zhang

Synthesis of enzyme imitation molecular imprinted nanocapsules catalyzing organophosphorus pesticide hydrolysis (2014-2015)

Synthesis of multi-function hollowed nanoparticles for gene delivery (2013-2014)

One-step synthesis of reactant-product-dual-template imprinted capsules as phosphotriesterase mimetic enzymes for pesticide elimination. (2012-2013)

PROFESSIONAL AFFILIATIONS

American Chemical Society, The Electrochemical Society, American Physical Society

Python Software Foundation