

Ruiyu Wang

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RESEARCH INTERESTS

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

SKILLS

VASP, Quantum-Espresso, GROMACS, Gaussian 09, CP2k, Chemoffice
C, C++, Python, Linux
Machine Learning

EDUCATION

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

- *Structure, Dynamics and chemistry of water near water/oxide interfaces.*
- Supervisor: [Prof. Eric Borguet](#), [Dr. Vincenzo Carnevale](#)

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

- *Synthesis and mechanism study of enzyme imitation molecular imprinted nanocapsule for catalyzing hydrolysis of organophosphorus pesticide.*
- Supervisor: Prof. Tianying Guo

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

- *Preparation of a functional polymersome.*
- Supervisor: Prof. Tianying Guo

PUBLICATIONS

(At Temple University)

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. In preparation, 2021.

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. *Submitted*, 2021. ([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. *European Polymer Journal* **2019**, 110, 1-8. ([link](#))

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. *European Polymer Journal* **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. *Journal of Applied Polymer Science* **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. *Journal of Materials Chemistry 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 Advances* **2014**, 4(16), 7881-7884

AWARDS

Doctoral Dissertation Completion grant,

College of Science and Technology(CST) Outstanding Research Assistant (RA) Award,

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

PROFESSIONAL AFFILIATIONS

American Chemical Society, The Electrochemical Society, American Physical Society

Python Software Foundation

PRESENTATIONS

CONFERENCE

On the Role of α -Alumina in the Origin of Life: Surface Driven Assembly of Amino Acids (ACS student travel awards)

Water hydrophilic behavior at aqueous/alumina interfaces

ACS Spring 2021 conference, 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; Temple University, USA. 2019

RESEARCH PROJECTS

(At Temple University)

Supervisor: Eric Borguet, Vincenzo Carnevale

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 (2018-2021)

Other Collaborators: Stefan Piontek, Richard C. Remsing, Mark DelloStritto, Tim Marshall

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)