

# Ruiyu Wang

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## RESEARCH INTERESTS

Molecular Dynamics Simulations  
Water/oxide interfaces  
Free Energy Calculation  
Vibrational Spectra Prediction  
Machine Learning for ab initio MD simulations

## EDUCATION

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

- *Structure, Dynamics and chemistry of water near water/oxide interfaces.*
- Supervisor: Eric Borguet, 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: Tianying Guo

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

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

## PUBLICATIONS

(At Temple University)

**Wang, R.**, Klein M., Carnevale V. & Borguet E. (2019) Investigation of water/solid interfaces by molecular dynamic simulations (in preparation)

**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  $\alpha$ -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

## SKILLS

VASP, Quantum-Espresso, GROMACS, Gaussian 09, CP2k, Chemoffice  
C, C++, Python, Linux  
Chemistry lab techniques

## AWARDS

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

### CONFERENCE

*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  $\alpha$ -alumina (0001)/water interface*  
ACS YCC Poster Session and Grad School/Career Fair, Philadelphia. 2018

*Ion adsorption and water behavior near  $\alpha$ -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  $\alpha$ -alumina(0001)/water interfaces for life origin (2019-)*

Other Collaborators: Richard C. Remsing

*Calculations of pKa by recently developed SCAN functional (2018-)*

Other Collaborators: Richard C. Remsing, Mark DelloStritto

*Dynamics, hydrogen bond structures and vibrational analysis at the neutral alumina (0001)/water interface (2018-2019)*

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-Supervisor: 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

Python Software Foundation