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 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

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 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-)
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