Personal Information

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Education

Sep. 2004—June 2009:

Ph.D. in Chemical Engineering under the direction of Professor **Xiaoning Yang**, State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing University of Technology, Nanjing, China

Sep. 2000—June 2004:

B.S. in Chemical Engineering, Nanjing University of Technology, Nanjing, China

Employment

Nov. 2011—Now:

Associate Professor, College of Chemistry and Chemical Engineering, Jiangxi Normal University, Nanchang, China

July 2011—Oct. 2011:

Assistant Professor, College of Chemistry and Chemical Engineering, Jiangxi Normal University, Nanchang, China

July 2009—June 2011:

Postdoctoral Research Fellow with Professor **Shuhua Li**, Institute of Theoretical and Computational Chemistry, Nanjing University, Nanjing, China

Grants and Projects

1. Stabilization Mechanism of Metal Nanoparticles in Imidazolium-based Ionic Liquids from Multi-scale Simulation Study, **Funded by the National Natural Science Foundation of China (No. 21463011)**, ***Principal Investigator***, From Jan. 01, 2015 to Dec. 30, 2018.
2. Diffusion mechanism of carbon doxide in zeolitic imidazolate framework membranes from free energy calculations, **Funded by the National Natural Science Foundation of China (No. 21306070)**, ***Principal Investigator***, From Jan. 01, 2014 to Dec. 30, 2016.
3. Separation mechanism of carbon dioxide gas mixtures in zeolitic imidazolate framework from a QM/MM study, **Funded by the Natural Science Foundation of Jiangxi Province (No. 20151BAB203014)**, ***Principal Investigator***, From Jan. 01, 2015 to Dec. 30, 2017.

Research Experience

(1) Structures of confined fluids in the various external fields (prior work, MM)

Nonlocal free-energy density functional theory (NLDFT) was employed to investigate structures of binary fluid mixtures (i.e. Yukawa and Lennard-Jones model) near the solid surfaces or membrane. Some effective adjustments in the long-range dispersion term were made to improve the accuracy of NLDFT approach. Meanwhile, grand canonical Monte Carlo (GCMC) simulations were carried out to test the validity of the NLDFT approach.

(2) Melting transition of bimetallic nanoparticles (prior work, MM)

The basic thermodynamics and structural properties of monometallic and bimetallic nanoparticles were studied by using molecular dynamics simulation with the semi-empirical many-body potentials. My main interest is to understand the relationship between the melting point and size, composition, and atomic arrangement and the nature of melting transition of nanoparticle. In addition, dynamical structure evolution processes were also studied.

(3) Solvation of nanoparticle in explicit solvent (prior work, MM)

The solvation free enregies of passivated nanoparticle with self-assembled monolayer in explicit solvent was calculated through the combination of molecular simulation with free energy perturbation (FEP) method. An effective fragment-based FEP was proposed to solve the difficulties of sampling near the ending thermodynamics windows.

(4) Structure of large water clusters in gas phase and confined in MOFs (prior work, QM, QM/MM)

Based on the generalized energy-based fragment (GEBF) approach proposed by Prof. Shuhua Li, a modified Basin-hopping method was applied to search low-lying structures of water clusters at the B3LYP and MP2 Level. On the other hand, the combination of GEBF method and OPLS force field (i.e. QM/MM method) was used to investigate the confined structures of neutral and protonated water clusters in MOFs.

(5) Adsorption mechanism of CO_2 in MOFs (prior work, QM, MM)

GCMC simulations and First-principles caculations was used to explain that an amide-inserted MOF (NJU-Bai3) presents

high storage and high selectivity toward CO_2. We revealed that amide groups can significantly enhance the CO2 binding ability and selectivity of MOFs at a molecular-level.

(6) Hydrogen bond (HB) dynamics and vibrational spectra of water (or ionic liquids) at the liquid-solid interfaces (current work, MM)

Detailed HB dynamics and vibrational spectra studied in our work provide insights into the unique behavior of water molecules at the interface of monolayer-protected Au nanoparticle (MPAN). More interestingly, our simulations reveal at a molecular level the relationship of solvation structure and dynamics, HBs, and IR spectra of hydration water molecules around the MPAN.

Skills

Operating Systems: DOS, Windows, Linux/Unix

Modelling Software: Tinker, Gaussian, Lammps, Material studio, VMD, and so on.

Programming: Fortran 77/95, Matlab

(1) I have written NLDFT, Canonical MC, Grand Canonical MC, MD (NVT and NPT), Basin-hopping codes and many postprocessing programs (RDF, MSD, H-bond dynamics, IR spectra, free energy perturbation).

(2) I can modify Tinker software to meet various research goals, and combine the Tinker and Gaussian softwares to construct the QM/MM method.

Main Publications

1. Guobing Zhou, **Zhen Yang**,* Fangjia Fu, Yiping Huang, Xiangshu Chen,* Zhanghui Lu, Na Hu, Molecular-level understanding of solvation structures and vibrational spectra of ethylammonium nitrate ionic liquid around single-walled carbon nanotubes, ***Ind. Eng. Chem. Res.***, **2015**, **Accepted**.
2. Guobing Zhou, **Zhen Yang**,* Fangjia Fu, Na Hu, Xiangshu Chen,* Duanjian Tao, Melting mechanism and structure evolution of Au nanofilms explored by molecular dynamics simulations, ***Chin. J. Chem. Phys.***, **2015**, **Accepted**.
3. **Zhen Yang**,* Yunzhi Li, Guobing Zhou, Xiangshu Chen,* Duanjian Tao, Na Hu, Molecular dynamics simulations of hydrogen bond and far-infrared spectra of hydration water molecules around the mixed monolayer-protected Au nanoparticle, ***J. Phys. Chem. C***, **2015**, 119, 1768.
4. **Zhen Yang**,* Hao Lin, Tian Gui, Rongfei Zhou, Xiangshu Chen,* Infrared spectroscopy of N-methylacetamide in water from high-level QM/MM calculations, ***Chin. Chem. Lett.***, **2014**, 25, 107.
5. Yunzhi Li, **Zhen Yang**,* Na Hu, Rongfei Zhou, Xiangshu Chen,* Insights into hydrogen bond dynamics at the interface of the charged monolayer-protected Au nanoparticle from molecular dynamics simulation, ***J. Chem. Phys.***, **2013**, 138, 184703.

6. Baishu Zheng, **Zhen Yang**, Junfeng Bai,* Yizhi Li, Shuhua Li,* High and selective CO_2 capture by two mesoporous acylamide-functionalized rht-type metal-organic frameworks, ***Chem. Commun.***, **2012**, 48, 7025-7027. (**Back Cover**)

7. Jingui Duan, **Zhen Yang**, Junfeng Bai,* Baishu Zheng, Yizhi Li, Shuhua Li,* Highly selective CO_2 capture of an *agw*-type metal–organic framework with inserted amides: experimental and theoretical studies, ***Chem. Commun.***, **2012**, 48, 3058-3060. (**Back Cover**)

8. **Zhen Yang**, Shugui Hua, Weijie Hua, Shuhua Li,* Structures of neutral and protonated water clusters confined in predesigned Hosts: A quantum mechanical/molecular mechanical study, ***J. Phys. Chem. B***, **2011**, 115, 8249-8256.

9. Qiu Du, **Zhen Yang**, Nannan Yang, Xiaoning Yang,* Coarse-grained model for perfluorocarbons and phase equilibrium simulation of perfluorocarbons/CO_2 mixtures, ***Ind. Eng. Chem. Res.***, **2010**, 49, 8271-8278.

10. **Zhen Yang**, Shugui Hua, Weijie Hua, Shuhua Li,* Low-lying structures and stabilities of large water clusters: Investigation based on the combination of the AMOEBA potential and generalized energy-based fragmentation approach, ***J. Phys. Chem. A***, **2010**, 114, 9253-9261.

11. **Zhen Yang**, Xiaoning Yang,* Zhijun Xu, Molecular simulations of structures and solvation free energies of passivated gold nanoparticles in supercritical CO_2, ***J. Chem. Phys.***, **2010**, 133, 094702.

12. Zhijun Xu, Xiaoning Yang,* **Zhen Yang**, A molecular simulation probing of structure and interaction for supramolecular sodium dodecyl sulfate/single-wall carbon nanotube assemblies, ***Nano. Lett.***, **2010**, 10, 985-991. (**Highlight Paper**)

13. **Zhen Yang**, Xiaoning Yang,* Zhijun Xu, Structural evolution of Pt-Au nanoalloys during heating process: comparison of random and core-shell orderings, ***Phys. Chem. Chem. Phys.***, **2009**, 11, 6249-6255.

14. **Zhen Yang**, Xiaoning Yang,* Zhijun Xu, Molecular dynamics simulation of the melting behavior of Pt-Au nanoparticles with core-shell structure, ***J. Phys. Chem. C***, **2008**, 112, 4937-4947. (**Cover Paper**)

15. Zhijun Xu, Xiaoning Yang,* **Zhen Yang**, On the mechanism of surfactant adsorption on solid surface: Free-energy investigations, ***J. Phys. Chem. B***, **2008**, 112, 13802-13811.

16. **Zhen Yang**, Xiaoning Yang,* Zhijun Xu, Structure of hard-core Yukawa fluid mixtures near a semi-permeable membrane: A density functional study, ***J. Membr. Sci.***, **2008**, 320, 381-389.

17. Zhijun Xu, Xiaoning Yang,* **Zhen Yang**, Adsorption and self-assembly of surfactant/supercritical CO_2 systems in confined pores: A molecular dynamics simulation, ***Langmuir***, **2007**, 23, 9201-9212.