



Department: School of Chemistry and Molecular Engineering

Professional field: Theoretical and Computational Chemistry

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Profile

2007.9-2011.7, B.S., Applied Chemistry, East China University of Science and Technology

2011.9-2016.6, Ph.D., Industrial Catalysis, East China University of Science and Technology

(Adviser: Prof. Xue-Qing Gong)

2016.7-2019.10, Postdoctoral Associate, University of Minnesota - Twin Cities (Advisers: Prof. Donald G. Truhlar and Prof. Laura Gagliardi)

2019.11-Present, Distinguished Research Fellow, East China University of Science and Technology

Research Field

- Developing and applying combined quantum mechanical and molecular mechanical (QM/MM) methods for complex systems, especially metal-organic frameworks (MOFs)

- Force field parametrization

- Surface chemistry, with a special emphasis on defects

- Computational catalysis and photocatalysis with MOFs, metals, and metal oxides

- Computational simulation of solid-state NMR spectra

Research results and selected published papers

- COMPUTATIONAL PROGRAM PACKAGE (CO-AUTHORED)

QMMM (<https://comp.chem.umn.edu/qmmm/>)

Description: QMMM is a computer program for performing single-point calculations (energies, gradients, and Hessians), geometry optimizations, and molecular dynamics using combined quantum mechanics (QM) and molecular mechanics (MM) methods.

- BOOK CHAPTER

“Photo-Induced Charge Separation and Photoredox Catalysis in Cerium-Based Metal-Organic Frameworks,” Xin-Ping Wu and Donald G. Truhlar*, in Computational Photocatalysis: Modeling of Photophysics and Photochemistry at Interfaces, edited by D. Kilin, S. Kilina, and Y. Han (American Chemical Society Symposium Series, Washington, DC, 2019), chapter 14, pp 309–326. (ISBN13: 9780841235540; eISBN: 9780841235533; DOI: 10.1021/bk-2019-1331)

- JOURNAL ARTICLES (*: CORRESPONDING AUTHOR; #: CO-FIRST AUTHOR)

1. Interactions of Oxide Surfaces with Water Revealed with Solid-State NMR Spectroscopy

Junchao Chen#, Michael A. Hope#, Zhiye Lin, Meng Wang, Tao Liu, David M. Halat, Yujie Wen, Teng Chen, Xiaokang Ke, Pieter C. M. M. Magusin, Weiping Ding, Xifeng Xia, **Xin-Ping Wu***, Xue-Qing Gong, Clare P. Grey*, and Luming Peng*

J. Am. Chem. Soc. 142, 11173–11182 (2020)

2. Polar Surface Structure of Oxide Nanocrystals Revealed with Solid-State NMR Spectroscopy

Junchao Chen#, **Xin-Ping Wu#***, Michael A. Hope#, Kun Qian, David M. Halat, Tao Liu, Yuhong Li, Li Shen, Xiaokang Ke, Yujie Wen, Jia-Huan Du, Pieter C. M. M. Magusin, Subhradip Paul, Weiping Ding, Xue-Qing Gong, Clare P. Grey*, and Luming Peng*

Nat. Commun. 10, 5420 (2019)

3. Multilink F* Method for Combined Quantum Mechanical and Molecular Mechanical Calculations of Complex Systems

Xin-Ping Wu*, Laura Gagliardi, and Donald G. Truhlar*

J. Chem. Theory Comput. 15, 4208–4217 (2019)

4. Cerium Metal-Organic Framework for Photocatalysis

Xin-Ping Wu*, Laura Gagliardi*, and Donald G. Truhlar*

J. Am. Chem. Soc. 140, 7904–7912 (2018)

5. Distinguishing Faceted Oxide Nanocrystals with 17O Solid-State NMR Spectroscopy

Yuhong Li#, **Xin-Ping Wu#**, Ningxin Jiang, Ming Lin, Li Shen, Haicheng Sun, Yongzheng Wang, Meng Wang, Xiaokang Ke, Zhiwu Yu, Fei Gao, Lin Dong, Xuefeng Guo, Wenhua Hou, Weiping Ding, Xue-Qing Gong*, Clare P. Grey, and Luming Peng*

Nat. Commun. 8, 581 (2017)

6. The Critical Role of Water in the Ring Opening of Furfural Alcohol to 1,2-Pentanediol

Rongfang Ma#, **Xin-Ping Wu#**, Tao Tong, Zheng-Jiang Shao, Yanqin Wang*, Xiaohui Liu, Qineng Xia*, and Xue-Qing Gong*

ACS Catal. 7, 333–337 (2017)

7. High-Performance PdNi Nanoalloy Catalyst in situ Structured on Ni Foam for Catalytic

Deoxygenation of Coalbed Methane: Experimental and DFT Studies

Qiaofei Zhang#, **Xin-Ping Wu#**, Yakun Li, Ruijuan Chai, Guofeng Zhao*, Chunzheng Wang, Xue-Qing Gong*, Ye Liu, and Yong Lu*

ACS Catal. 6, 6236–6245 (2016)

8. Clustering of Oxygen Vacancies at CeO₂(111): Critical Role of Hydroxyls

Xin-Ping Wu and Xue-Qing Gong*

Phys. Rev. Lett. 116, 086102 (2016)

9. Unique Electronic and Structural Effects in Vanadia/Ceria-Catalyzed Reactions

Xin-Ping Wu and Xue-Qing Gong*

J. Am. Chem. Soc. 137, 13228–13231 (2015)