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个人简介

2007.9-2011.7，华东理工大学，应用化学（材料），本科

2011.9-2016.6，华东理工大学，工业催化，博士研究生

2016.7-2019.10，美国明尼苏达大学，博士后

2019.11- 今，华东理工大学，计算化学中心、工业催化研究所，特聘研究员

研究方向

- 针对复杂体系，特别是金属有机框架（MOF）材料，开发量子力学和分子力学组合（QM/MM）方法
- 分子力场拟合
- 表面化学，重点关注缺陷
- MOF、金属、金属氧化物等催化及光催化材料的理论计算研究
- 固体核磁谱图的理论模拟

研究成果及主要发表文章

- 计算程序 （参与开发）

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

介绍：QMMM 是采用量子力学（QM）和分子力学（MM）组合方法进行单点（能量、梯度、海森）、结构优化及分子动力学计算的程序。

- 专著章节

“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)

- 期刊论文 （*： 通讯作者； #： 共同第一作者）

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)