

Zhi-Jian Zhao (赵志坚)

Male, Birthday Apr. 9 1983, Chinese

zizhao@tju.edu.cn



Highlights

- Extensive theoretical studies on **heterogeneous catalysis** and **polymer science**
- Experienced in Density Functional Theory (**DFT**), genetic algorithm based global optimization, molecular dynamics (**MD**) methods, micro-kinetic modeling and kinetic Monte Carlo (**kMC**) simulation
- Strong programming ability with **C, Python, Qt**, etc, including simple UI design
- Publications: **20 publications**, total **IF = 60**, H-index = 7

Skills

Programming Experienced in **C, Python, Qt**; familiar with C++ and Fortran
Software Experienced in **VASP, ASE, GPAW**; familiar with Gaussian, Turbomole, , Gromacs, Tinker
Language Skilled in **English, Chinese(native)**; basic in German

Education

- 2008 - 2012** Doctor, Department Chemie, *Technische Universität München*, Garching, Bavaria, Germany.
 ➤ **Passed with Distinction**
- 2006 - 2008** Master, Department of Chemistry, *Zhejiang University*, Hangzhou, Zhejiang, China.
 ➤ **Over-all GPA: 3.80/4.00** **Major GPA: 3.97/4.00**
- 2002 - 2006** Bachelor, Department of Chemistry, *Zhejiang University*, Hangzhou, Zhejiang, China.
 ➤ **Over-all GPA: 3.80/4.00** **Major GPA: 3.91/4.00** **Ranked 4th in about 90**

Work Experience

2012.10-2012.12, Technical University of Munich, Department of Chemistry, supervisor Prof. N. Rösch, PostDoc

2013.01-2014.10, Purdue University, School of Chemical Engineering, supervisor Prof. J. Greeley, PostDoc

2014.10-2015.10, Stanford University, School of Chemical Engineering, and SLAC National Accelerator Laboratory, and supervisors Dr. F. Studt and Prof. J. Nørskov, PostDoc

2015.10-present, Tianjin University, School of Chemical Engineering and Technology, **Associate Professor**

Research Experience

- 2013 – 2014** Support effect of the water-gas shift (WGS) reactions (**Interface modeling, DFT**)
- Under supervision of **Prof. Jeffrey Greeley** at Purdue University
 - Joint project with **Prof. Nicholas Delgass** and **Prof. Fabio Ribeiro** at Purdue University
 - Try to understand the role of support on the activity of WGS reactions
 - Build numerical solution of reaction kinetics with plug flow reactor model
- 2013 – 2014** Global optimization with genetic algorithm (**Algorithm development, DFT**)

- Under supervision of **Prof. Jeffrey Greeley** at Purdue University
- Try to understand Pt alloys oxidation reactions
- Written in Python within the framework of Atomic Simulation Environment
- 2014** Selective oxidation of Glycerol via Bi-Pt catalysts (**DFT**)
 - Under supervision of **Prof. Jeffrey Greeley** at Purdue University
 - In corporation with **Prof. Varma** at Purdue University
 - Successfully explained different selectivity with different contain of Bi
- 2010 – 2011** Pd catalyst leaching process in Heck reaction (**Thermodynamics, DFT**)
 - Under supervision **Prof. Notker Rösch** at Technische Universität München
 - Joint project with **Prof. Jun Li** at Tsinghua University, P.R. China
 - Direct theoretical evidence for loss of catalyst by interactions from the reactant
- 2008 – 2012** Selective ring opening of cyclic hydrocarbons during fuel upgrading (**Kinetics, DFT, kMC**)
(Doctor thesis)
 - Under supervision **Prof. Notker Rösch** at Technische Universität München
 - Cooperated with **Prof. Johannes Lercher** at Technische Universität München
 - Clarified the mechanism of ethylene conversion over Pt(111)
 - Explained the particle size effect of ring opening reactions on supported metal catalysts
 - Designed a program for parallel calculation of similar tasks
- 2005 – 2008** Diffusion process of drugs in controlled release materials (**MD**)
(Bachelor, Master thesis)
 - Under supervisor **Prof. Qi Wang** at Zhejiang University
 - Explained the different diffusion mechanisms for particles with different size in the controlled release materials
 - Designed a series of programs for automatic calculation and data analysis

Honors and Awards

- 2015** 天津市青年千人
- 2007 - 2008** Excellent Master Student of Zhejiang Province (**Top 1%**, 浙江省优秀硕士毕业生)
- 2006 - 2007** **Chu Kochen** award (**Top 0.1%**, 浙江大学竺可桢奖学金)
 - Highest honor for students in Zhejiang University
 - Written in the history of the university
 - Annually award top 4 in all masters (ca. 8000) of Zhejiang University
- 1st prize** for Excellent Student Award of Zhejiang University (**Top 5%**)
- 2005 - 2006** Excellent Undergraduate Student and Excellent Bachelor Thesis (**Top 5%**)
- 2002 - 2006** 3 / 3 times Excellent Student Award, including one time
3 / 3 times Excellent Academic Award of Zhejiang University
- 1990 - 2008** 25 / 25 times Excellent Student
2005

Publications

1. **Z.-J. Zhao**, C.-c. Chiu, J.-L. Gong, Molecular Understandings on Heterogeneous Catalytic Dehydrogenation of Light Alkanes, **2015**, *Chem. Sci.* 4403 (**Front cover**)

2. **Z.-J. Zhao**, J. Greeley, Identification of surface intermediates during ethylidyne formation on Pt (111) by calculation of infrared intensities and deuterium isotope shifts, *Surf. Sci.* **2015**, doi:10.1016/j.susc.2015.01.022 (*Invited*)
3. Z.-H. Zeng, M.K.Y. Chan, **Z.-J. Zhao**, J. Kubal, D.-X. Fan, J. Greeley, Towards First Principles-based Prediction of Highly Accurate Electrochemical Pourbaix Diagrams, *J. Phys. Chem. C* **2015**, DOI: 10.1021/acs.jpcc.5b03169
4. L. Li, J. Yan, T. Wang, **Z.-J. Zhao**, J. Zhang, J. Gong, N. Guan, Sub-10 nm rutile titanium dioxide nanoparticles for efficient visible-light-driven photocatalytic hydrogen production, *Nat. Comm.* **2015**, 6, 5881.
5. H. Mistry, R. Reske, Z. Zeng, **Z.-J. Zhao**, J. Greeley, P. Strasser, B. R. Cuenya, Exceptional size-dependent activity enhancement in the electroreduction of CO₂ over Au nanoparticles, *J. Am. Chem. Soc.* **2014**, 136, 16473.
6. H. Yildirim, A. Kinaci, **Z.-J. Zhao**, M.K.Y. Chan, J. Greeley, First Principles Analysis of Defect-Mediated Li Adsorption on Graphene, *ACS Appl. Mater. Inter.*, **2014**, 6, 21141.
7. H. Shi, Y.-C. Liu, **Z.-J. Zhao**, M. Miao, T. Wu, Qi. Wang, Reactivity of the defective rutile TiO₂ (110) surfaces with two bridging oxygen vacancies: water as a probe molecule, *J. Phys. Chem. C* **2014**, 118, 20257
8. D. Luo, **Z.-J. Zhao**, L. Zhang, Q. Wang, J. Wang, X. Wang, On the structure of molecularly imprinted polymers by modifying charge on function groups through molecular dynamics simulations, *Mol. Simulat.*, **2014**, 40, 431
9. **Z.-J. Zhao**, L.V. Moskaleva, N. Rösch, Formation of *n*-hexane from methylcyclopentane via a metallacyclobutane intermediate at step sites of Pt surfaces: Mechanism from first-principles calculations, *J. Catal.* **2013**, 299, 146
10. **Z.-J. Zhao**, L.V. Moskaleva, N. Rösch, Ring-opening reactions of methylcyclopentane over M (M = Pd, Pt, Rh, and Ir) catalysts: A mechanistic study from first-principles calculations, *ACS Catal.* **2013**, 3, 196
11. **Z.-J. Zhao**, L.V. Moskaleva, N. Rösch, Tuning the selectivity for methylcyclopentane ring-opening reactions over Pt catalysts: A mechanistic study from first-principle calculations, *J. Catal.* **2012**, 285, 124
12. C.-R. Chang, **Z.-J. Zhao**, K. Köhler, A. Genest, J. Li, Notker Rösch, Theoretical investigations on Pd leaching in CO atmosphere, *Catal. Sci. Technol.* **2012**, 2, 2238 (*Hot Article*)
13. H.A. Aleksandrov, L.V. Moskaleva, **Z.-J. Zhao**, D. Basaran, D. Mei, N. Rösch, Ethylene conversion to ethylidyne on Pd(111) and Pt(111). A first-principles-based kinetic Monte Carlo study, *J. Catal.* **2012**, 285, 187
14. D. Basaran, H.A. Aleksandrov, Z.-X. Chen, **Z.-J. Zhao**, N. Rösch, Model decomposition of ethylene on Pd(111), Pt(111), Ni(111) and Rh(111): a periodic DFT study, *J. Mol. Catal. A: Chemical*, **2011**, 344, 37
15. **Z.-J. Zhao**, L.V. Moskaleva, H.A. Aleksandrov, D. Basaran, N. Rösch, Ethylidyne Formation from Ethylene over Pt(111): A mechanistic Study from First-Principle Calculations, *J. Phys. Chem. C* **2010**, 114, 12190
16. L.V. Moskaleva, H.A. Aleksandrov, D. Basaran, **Z.-J. Zhao**, N. Rösch, Ethylidyne Formation from Ethylene over Pd(111): Alternative Routes from a Density Functional Study, *J. Phys. Chem. C* **2009**, 113, 15373
17. **Z.-J. Zhao**, Q. Wang, L. Zhang, T. Wu, Structured Water and Water-Polymer Interactions in Hydrogels of Molecularly Imprinted Polymers, *J. Phys. Chem. B* **2008**, 112, 7515
18. **Z.-J. Zhao**, Q. Wang, L. Zhang, and Y.-C. Liu, A Different Diffusion Mechanism for Drug Molecules in Amorphous Polymers, *J. Phys. Chem. B* **2007**, 111, 4411
19. **Z.-J. Zhao**, Q. Wang, L. Zhang, Size Effect on Competition of Two Diffusion Mechanisms for Drug Molecules in Amorphous Polymers, *J. Phys. Chem. B* **2007**, 111, 13167
20. Y. Xiao, **Z.-J. Zhao**, I. Levett, J. Greeley, G. Xiao, A. Varma, An Experimental and Theoretical Study on Glycerol Selective Oxidation to Dihydroxyacetone via Bimetallic Bismuth-Platinum Catalysts, in preparation
21. **Z.-J. Zhao**, N. W. Delgass, F. H. Ribeiro, J. Greeley, et al. Understanding the Important Role of Interface in Heterogeneous Catalyst: Water-Gas Shift Model Reactions Over Au/MgO, in preparation
22. **Z.-J. Zhao**, J. Greeley, et al. Initial oxidation state of Pt alloy electrode: generic algorithm based global optimizing for complicated surface reconstructions, in preparation
23. **Z.-J. Zhao**, A. Genest, N. Rösch, Identification of surface intermediate via vibrational frequency analysis:

aperiodic DFT study, in preparation

Conferences and Schools

1. 2013 Spring Symposium of Catalysis Club of Chicago, 7.5.2013, Chicago, U.S.A., poster
2. 15th International Congress on Catalysis 2012, 1.7-6.7.2012, Munich, Germany, poster
3. 45. Jahrestreffen Deutscher Katalytiker (45th Annual Meeting of German Catalysis), 14.3-16.3.2012, Weimar, Germany, poster
4. H.A. Aleksandrov, L.V. Moskaleva, **Z.-J. Zhao**, D. Basaran, Z.-X. Chen, D. Mei, N. Rösch, Conversion of unsaturated hydrocarbons: A computational study, Abstracts of Papers, 242nd ACS National Meeting & Exposition, Denver, CO, United States, 28.8-1.9, **2011** (2011), FUEL-315.
5. International course "Introduction to kinetic Monte Carlo simulations" at Technische Universiteit Eindhoven, 29.8.-2.9.2011, Eindhoven, Netherlands
6. Energy and Materials from the Sun, 19.6.-23.6.2011, Kerkrade, Netherlands, poster
7. H.A. Aleksandrov, **Z.-J. Zhao**, D. Basaran, L.V. Moskaleva, Z.-X. Chen, D. Mei, N. Rösch, Mechanistic study of ethylene conversion to ethylidyne on M(111) (M = Pd, Pt) with DFT and kinetic Monte Carlo simulations, Preprints of Symposia - American Chemical Society, Division of Fuel Chemistry, **2010**, 55(1), 536.
8. Catalysis Emerging Challenges in Catalysis, 12.5.-19.5.2010, Porquerolles, France, poster
9. European Graduate School (EGS) on Sustainable Energy-The Molecular Approach, 2.9.-4.9.2009, Heeze, Netherlands; 7.4.-9.4.2010, Freising, Germany; 9.12.-11.12.2010, Nyborg, Denmark, poster