



Curriculum Vitae

Personal details

Name Tao
Surname Wang
Place and Date of Birth (mm/dd/yy) Shandong, P.R. China, 10/09/1986
Marital status Married to XiaoHong Guo, one son
E-mail tao.wang@ens-lyon.fr or tommy0686@163.com

Education and research experience

10/01/2015 – present **Postdoctoral**, Ecole Normale Supérieure of Lyon, Lyon, France
Advisor: Prof. Philippe Sautet
Topic: Theoretical Investigations of Alcohols Selective Aminations on Heterogeneous Catalysts by using DFT based micro-kinetics

07/07/2015 – 09/30/2015 **Postdoctoral**, Leibniz-Institute for Catalysis at the University of Rostock, Rostock, Germany

10/01/2012 – 07/06/2015 **Research Doctorate**, Leibniz-Institute for Catalysis at the University of Rostock, Rostock, Germany
Topic: About CO and H₂ Activation Mechanisms on Fe and Mo₂C Catalysts on the Basis of Density Functional Theory Computation and Ab Initio Atomistic Thermodynamics
Supervisor: Prof. Haijun Jiao

07/01/2012-09/30/2012 **Research intern**, Synfuels China Co. Ltd., Beijing, China

09/01/2009 – 06/30/2012 **Master of Physical Chemistry**, Institute of Coal Chemistry, Chinese Academy of Science, Taiyuan, China & Synfuels China Co. Ltd., Beijing, China
Topic: Theoretical Study of Stability and Catalysis Activity of Hydro-treating Catalyst Surfaces
Supervisor: Prof. Haijun Jiao (Thousand talents plan professor of SXICC)

Award

-
- 07/2012 Excellent Master Thesis of Shanxi Province
- 10/2012 Leibniz Scholarship in Leibniz Institute for Catalysis
-

Working experience

-
- 07/2012-10/2012 Research intern, Synfuels China Co. Ltd., Beijing, China
-

Relevant skills

Proficient with the operation of VASP, CASTEP, DMol, and Gaussian software packages for ab initio first principle calculations of solid surface properties and related reaction mechanisms as well as DFT based mean field micro-kinetics modeling.

Excellent ability with MS Office, Origin, experienced in the use of SciFinder, Chemdraw etc and various graphic application tools.

Familiar with the compile of simple scripts for assisting calculations with Python programming language

List of Publications

- [33] Wang, T.; Michel, C.; Sabbe, M.; Pera-Titus, M.; Sautet, P. "Alcohol Selective Amination Catalysts Screening: A Conjoint Experimental and DFT based Micro-kinetics investigation" **2017, to be submitted.**
- [32] Wang, T.; Michel, C.; Sabbe, M.; Pera-Titus, M.; Sautet, P. "An Efficient Way to Identify Active Catalyst for Alcohol Dehydrogenation to Carbonyl Compound" **2017, to be submitted.**
- [31] Wang, T.; Michel, C.; Pera-Titus, M.; Sautet, P. "How can we Control the Nitridation of Transition Metal Surfaces? catalysts? Avoid?" **2017, to be submitted.**
- [30] Zhang, J.; Wang, T.; Liu, P.; Liao, Z. H.; Liu, S. H.; Zhuang, X. D.; Chen, M. W.; Zschech, E.; Feng, X. L. "Efficient Hydrogen Production on MoNi₄ Electrocatalysts with Fast Water Dissociation Kinetics". *Nature Commu.* **2017, under review** (minor revision).
- [29] Tian, X.-X.; Wang, T.; Jiao, H. "Mechanism of Coverage Dependent CO Adsorption and Dissociation on the Mo(100) Surface". *Phys. Chem. Chem. Phys.* **2017, 19, 2186-2192.**
- [28] Tian, X.-X.; Wang, T.; Yang, Y.; Li, Y.-W.; Wang, J.; Jiao, H. "About Copper Promotion in CH₄ Formation from CO Hydrogenation on Fe(100): A Density Functional Theory Study". *Appl. Catal. A: Gen.* **2017, 530, 83-92.**
- [27] Zhang, J.; Wang, T.; Liu, P.; Liu, S. H.; Dong, R. H.; Zhuang, X. D.; Chen, M. W.; Feng, X. L. "Engineering Water Dissociation Sites in MoS₂ Nanosheets for Accelerated Electrocatalytic Hydrogen Production". *Energy Environ. Sci.* **2016, 9, 2789-2793.**
- [26] Zhang, J.; Wang, T.; Pohl, D.; Rellinghaus, B.; Dong, R. H.; Liu, S. H.; Zhuang, X. D.; Feng, X.

- L. "Interface Engineering of MoS₂/Ni₃S₂ Heterostructures for Highly Enhanced Electrochemical Overall-Water-Splitting Activity". *Angew. Chem. Int. Ed.* **2016**, *55*, 6702-6707.
- [25] **Wang, T.**; Tian, X.-X.; Yang, Y.; Li, Y.-W; Wang, J.; Beller, M.; Jiao, H. "Surface Morphology of Orthorhombic Mo₂C Catalyst and High Coverage Hydrogen Adsorption" *Surf. Sci.* **2016**, *651*, 195-202.
- [24] **Wang, T.**; Tian, X.-X.; Yang, Y.; Li, Y.-W; Wang, J.; Beller, M.; Jiao, H. "Coverage-Dependent N₂ Adsorption and Its Modification of Iron Surfaces Structures." *J. Phys. Chem. C* **2016**, *120*, 2846-2854.
- [23] **Wang, T.**; Tian, X.-X.; Yang, Y.; Li, Y.-W; Wang, J.; Beller, M.; Jiao, H. "Structures of Seven Molybdenum Surfaces and Their Coverage Dependent Hydrogen Adsorption." *Phys. Chem. Chem. Phys.* **2016**, *18*, 6005-6012.
- [22] **Wang, T.**; Tian, X.-X.; Yang, Y.; Li, Y.-W; Wang, J.; Beller, M.; Jiao, H. "Co-adsorption and Mutual Interaction of nCO+mH₂ on the Fe(110) and Fe(111) Surfaces." *Catal. Today* **2016**, *261*, 82-92.
- [21] Liu, S.; Tian, X.-X.; **Wang, T.**; Wen, X.-D.; Li, Y.-W.; Wang, J.; Jiao, H. "Coverage Dependent Water Dissociative Adsorption on the Clean and O-Precovered Fe(111) Surfaces." *J. Phys. Chem. C* **2015**, *119*, 11714-11724.
- [20] **Wang, T.**; Tian, X.-X.; Yang, Y.; Li, Y.-W; Wang, J.; Beller, M.; Jiao, H. "Coverage Dependent Adsorption and Co-adsorption of CO and H₂ on the CdI₂-antitype Metallic Mo₂C(001) Surface." *Phys. Chem. Chem. Phys.* **2015**, *17*, 1907-1917.
- [19] Tian, X.-X.; **Wang, T.**; Yang, Y.; Li, Y.-W; Wang, J.; Jiao, H. "Surface Morphology of Cu Adsorption on Different Terminations of the Hägg Iron Carbide (χ -Fe₅C₂) Phase." *J. Phys. Chem. C* **2015**, *119*, 7371-7385.
- [18] Liu, S.; Tian, X.-X.; **Wang, T.**; Wen, X.-D.; Li, Y.-W.; Wang, J.; Jiao, H. "Coverage Dependent Water Dissociative Adsorption on Fe(110) from DFT Computation." *Phys. Chem. Chem. Phys.* **2015**, *17*, 8811-8821.
- [17] **Wang, T.**; Luo, Q.; Li, Y.-W; Wang, J. Beller, M.; Jiao, H. "Stable Surface Terminations of orthorhombic Mo₂C Catalysts and Their CO Activation Mechanisms." *Appl. Catal. A: Gen.* **2014**, *478*, 146-156.
- [16] **Wang, T.**; Li, Y.-W.; Wang, J.; Beller, M.; Jiao, H. "Dissociative Hydrogen Adsorption on the Hexagonal Mo₂C Phase at High Coverage." *J. Phys. Chem. C* **2014**, *118*, 8079-8089.
- [15] **Wang, T.**; Li, Y.-W; Wang, J.; Beller, M.; Jiao, H. "High Coverage CO Adsorption and Dissociation on the Orthorhombic Mo₂C(100) Surface." *J. Phys. Chem. C* **2014**, *118*, 3162-3171.
- [14] **Wang, T.**; Tian, X.-X.; Li, Y.-W; Wang, J.; Beller, M.; Jiao, H. "Coverage-Dependent CO Adsorption and Dissociation Mechanisms on Iron Surfaces from DFT Computations." *ACS Catal.* **2014**, *4*, 1991-2005.
- [13] **Wang, T.**; Wang, S. G.; Luo, Q.; Li, Y.-W; Wang, J.; Beller, M.; Jiao, H. "Hydrogen Adsorption Structures and Energetics on Iron Surfaces at High Coverage." *J. Phys. Chem. C* **2014**, *118*,

4181-4188.

- [12] **Wang, T.**; Tian, X.-X.; Li, Y.-W.; Wang, J.; Beller, M.; Jiao, H. "High Coverage CO Activation Mechanisms on Fe(100) from Computations." *J. Phys. Chem. C* **2014**, *118*, 1095-1101.
- [11] Tian, X.-X.; **Wang, T.**; Yang, Y.; Li, Y.-W.; Wang, J.; Jiao, H. "Copper Promotion in CO Adsorption and Dissociation on the Fe(100) Surface." *J. Phys. Chem. C* **2014**, *118*, 20472-20480.
- [10] Tian, X.-X.; **Wang, T.**; Yang, Y.; Li, Y.-W.; Wang, J.; Jiao, H. "Adsorption Structures and Energies of Cu_n Clusters on the Fe(110) and Fe₃C(001) Surfaces." *J. Phys. Chem. C* **2014**, *118*, 21963-21974.
- [9] Tian, X.-X.; **Wang, T.**; Yang, Y.; Li, Y.-W.; Wang, J.; Jiao, H. "Structures and Energies of Cu_n Clusters on Fe and Fe₃C Surfaces from Density Functional Theory Computation". *Phys. Chem. Chem. Phys.* **2014**, *16*, 26997-2701.
- [8] Liu, S. L.; Tian, X.-X.; **Wang, T.**; Wen, X.-D.; Li, Y.-W.; Wang, J.; Jiao, H. "High Coverage Water Aggregation and Dissociation on Fe(100) – A Computational Analysis" *J. Phys. Chem. C* **2014**, *118*, 26139-26154.
- [7] Luo, Q.; **Wang, T.**; Beller, M.; Jiao, H. "Molybdenum Carbide Catalysed Hydrogen Production from Formic Acid." *J. Power Sources* **2014**, *246*, 548-555.
- [6] Luo, Q.; **Wang, T.**; Beller, M.; Jiao, H. "Full Acrolein Hydrogenation on Ni(111)." *J. Phys. Chem. C* **2013**, *117*, 12715-12724.
- [5] Luo, Q.; **Wang, T.**; Beller, M.; Jiao, H. "Hydrogen Generation from Formic Acid Decomposition on Ni(211), Pd(211) and Pt(211)." *J. Mol. Catal. A* **2013**, *379*, 169-177.
- [4] Li, Q.; Li, Y. N.; **Wang, T.**; Wang, S. G.; Li, Y.-W.; Wang, J.; Jiao, H. "Electronic Structures and Energies of Fe₂(CO)_n (n=0–9)." *Chem. Phys. Chem.* **2013**, *14*, 1573-1576.
- [3] Li, Y. N.; Wang, S. G.; **Wang, T.**; Gao, R.; Geng, C. Y.; Li, Y.-W.; Wang, J.; Jiao, H. "Energies and Spin States of FeS^{0/-}, FeS₂^{0/-}, Fe₂S₂^{0/-}, Fe₃S₄^{0/-}, and Fe₄S₄^{0/-} Clusters." *Chem. Phys. Chem.* **2013**, *14*, 1182-1189.
- [2] **Wang, T.**; Wang, S. G.; Li, Y.-W.; Wang, J.; Jiao, H. "Adsorption Equilibria of CO Coverage on β-Mo₂C Surfaces." *J. Phys. Chem. C* **2012**, *116*, 6340-6348.
- [1] **Wang, T.**; Liu, X. W.; Wang, S. G.; Huo, C. F.; Li, Y.-W.; Wang, J.; Jiao, H. "Stability of β-Mo₂C Facets from ab initio Atomistic Thermodynamics." *J. Phys. Chem. C* **2011**, *115*, 22360-22368.

Conference participations

- [1] **Poster "Surface Stabilities and Coverage Dependent CO Activation Activity of Iron Catalyst"**

Tao Wang, Xin-xin Tian, Yong-Wang Li, Jianguo Wang, Matthias Beller and Haijun Jiao

At the "2014 CAMD Summer School on Electronic Structure Theory and Materials Design", Copenhagen, Denmark, August 16 – August 22, **2014**.

- [2] **Poster "Morphology of Mo₂C Catalyst under Carburization Condition and Coverage Dependent CO Activation Mechanism"**

Tao Wang, Xin-xin Tian, Matthias Beller and Haijun Jiao

At the "15th International Congress of Quantum Chemistry", Beijing, China, June 8-13, **2015**.

[3] **Oral "Surface Nitridation Mechanism of Ni Catalyst in Alcohols Aminations"**

Tao Wang, Carine Michel, Marc Pera-Titus, Philippe Sautet

At the "16th International Conference on Theoretical Aspects of Catalysis", Zakopane, Poland, June 19 – June 23, 2016.

[4] **Poster "An Efficient Theoretical Tool for Screening Promising Heterogeneous Catalysts in Alcohols Selective Aminations"**

Tao Wang, Alexandre S Dumon, Carine Michel, Marc Pera-Titus, Philippe Sautet

At the "16th International Congress on Catalysis" July 3 to 8, 2016 in Beijing, China.

[5] **Oral "Searching for Promising Catalysts in Alcohols Aminations by Using Scaling, BEP Relations and Micro-kinetics modeling"**

Tao Wang, Alexandre S Dumon, Carine Michel, Marc Pera-Titus, Philippe Sautet

At the "Satellite Symposium of 16th International Congress on Catalysis" July 10 to 12, 2016 in Xiamen, China.

References:

(1) Prof. Haijun Jiao, Email: haijun.jiao@catalysis.de

Leibniz Institute for Catalysis, Germany

(2) Prof. Philippe Sautet, Email: sautet@ucla.edu

French Academy of Science member; Associate Editor of ACS Catalysis; University of California Los Angeles, Chemical and Biomolecular Engineering department and CNSI

(3) Prof. Matthias Beller, Email: Matthias.Beller@catalysis.de

Leibniz Institute for Catalysis, Germany