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EDUCATION

09/2010-04/2015, PhD Candidate in Physical Chemistry, State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences, Dalian, China. Supervisor: Prof. Wei-Xue Li

09/2009 –07/2010, Basic training courses for PhD students, Department of Chemical Physics, University of Science and Technology of China, Hefei, China

09/2005 –07/2009, B.S. in Applied Physics, School of Physical Engineering, Zhengzhou University, Zhengzhou, China

PROFESSIONAL EXPERIENCE

09/2020 – present Research fellow in Department of Chemical Physics, School of Chemistry and Materials Science, University of Science and Technology of China, Hefei 230026, China

09/2019-08/2020, Postdoctoral research fellow in Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan. Work with Prof. Suljo Linic

04/2018-08/2019, Postdoctoral research fellow in Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan. Work with Prof. Bryan Goldsmith

05/2015-04/2018, Postdoc in Chemistry department, Eindhoven University of Eindhoven, Netherlands, Work with Prof. Emiel Hensen

RESEARCH INTERESTS

First-Principles Modeling, Molecular Simulation, Machine Learning
Surface science
Reaction mechanism
Syngas conversion chemistry
Environmental catalysis
Electrocatalysis

AWARDS

2013 Outstanding student, Chinese Academy of Sciences
2013 Awarded national scholarships
2014 Outstanding graduate student of DICP
2014 Pacemaker to merit student, Chinese Academy of Sciences
2014 Dean excellence award, Chinese Academy of Sciences
2015 Excellent Doctoral Scholarship of ZhuLiYueHua
2015 Excellent Graduate of Chinese Academy of Sciences

PUBLICATIONS (# co-first author, * corresponding authors)

BEFOR USTC (2011 - 2020)

40. First-Principles Microkinetics Simulations of Electrochemical Reduction of CO_2 over Cu Catalysts. Zijlstra, B.#; Zhang, X.#; ***Liu, J.-X.#***; Filot, I. A. W.; Zhou, Z.; Sun, S.; Hensen, E. J. M., *Electrochim. Acta* **2020**, *335*, 135665.
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38. Compensation between Surface Energy and hcp/fcc Phase Energy of Late Transition Metals from First-Principles Calculations. Lin, H.#; ***Liu, J.-X.#***; Fan, H.; Li, W.-X., *J. Phys. Chem. C* **2020**, *124*, 11005-11014.
37. Understanding the Impact of Defects on Catalytic CO Oxidation of LaFeO3-Supported Rh, Pd, and Pt Single-Atom Catalysts. Zhang, L.; Filot, I. A. W.; Su, Y. Q.; ***Liu, J. X.***; Hensen, E. J. M., *J. Phys. Chem. C* **2019**, *123*, 7290-7298.
36. Interplay between Site Activity and Density of bcc Iron for Ammonia Synthesis Based on First-Principles Theory. Zhang, B. Y.; Su, H. Y.; ***Liu, J. X.***; Li, W. X., *Chemcatchem* **2019**, *11*, 1928-1934.
35. Influence of Cobalt Crystal Structures on Activation of Nitrogen Molecule: A First-Principles Study. Zhang, B. Y.; Chen, P. P.; ***Liu, J. X.****; Su, H. Y.; Li, W. X.*, *J. Phys. Chem. C* **2019**, *123*, 10956-10966.
34. Surpassing the Single-Atom Catalytic Activity Limit through Paired Pt-O-Pt Ensemble Built from Isolated Pt_1 Atoms. Wang, H.#; ***Liu, J. X.#***; Allard, L. F.; Lee, S.; Liu, J.; Li, H.; Wang, J.; Wang, J.; Oh, S. H.; Li, W.; Flytzani-Stephanopoulos, M.; Shen, M.; Goldsmith, B. R.; Yang, M., *Nat. Commun.* **2019**, *10*, 3808.
33. A Theoretical Approach to Predict Stability of Supported Single-Atom Catalysts. Su, Y.-Q.; Wang, Y.; ***Liu, J.-X.***; Filot, I. A.; Alexopoulos, K.; Zhang, L.; Muravev, V.; Zijlstra, B.; Vlachos, D. G.; Hensen, E. J., *ACS Catal.* **2019**, *9*, 3289-3297.
32. Single Ru Sites-Embedded Rutile TiO_2 Catalyst for Non-Oxidative Direct Conversion of Methane: A First-Principles Study. Ma, X.; Sun, K.; ***Liu, J.-X.***; Li, W.-X.; Cai, X.; Su, H.-Y., *J. Phys. Chem. C* **2019**, *123*, 14391-14397.
31. Activity and Selectivity Trends in Electrocatalytic Nitrate Reduction on Transition Metals. ***Liu, J.-X.***; Richards, D.; Singh, N.; Goldsmith, B. R., *ACS Catal.* **2019**, *9*, 7052-7064.
30. Nitrogen-Doped Graphene Layers for Electrochemical Oxygen Reduction Reaction Boosted by Lattice Strain. Li, J.#; ***Liu, J.-X.#***; Gao, X.; Goldsmith, B. R.; Cong, Y.; Zhai, Z.; Miao, S.; Jiang, Q.; Dou, Y.; Wang, J.; Li, W.-X.; Song, Y., *J. Catal.* **2019**, *378*, 113-120.

29. Two-to-Three Dimensional Transition in Neutral Gold Clusters: The Crucial Role of Van Der Waals Interactions and Temperature. Goldsmith, B. R.; Florian, J.; ***Liu, J.-X.***; Gruene, P.; Lyon, J. T.; Rayner, D. M.; Fielicke, A.; Scheffler, M.; Ghiringhelli, L. M., *Phys. Rev. Mater.* **2019**, *3*, 016002.
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26. Transition Metal Doping of Pd (111) for the NO+CO Reaction. Zhang, L.; Filot, I. A.; Su, Y.-Q.; ***Liu, J.-X.***; Hensen, E. J., *J. Catal.* **2018**, *363*, 154-163.
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23. Optimum Particle Size for Gold-Catalyzed CO Oxidation. ***Liu, J.-X.***; Filot, I. A. W.; Su, Y.; Zijlstra, B.; Hensen, E. J. M., *J. Phys. Chem. C* **2018**, *122*, 8327-8340.
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20. Reconstruction of the Wet Chemical Synthesis Process: The Case of Fe_5C_2 Nanoparticles. Yao, S.; Yang, C.; Zhao, H.; Li, S.; Lin, L.; Wen, W.; ***Liu, J. X.***; Hu, G.; Li, W.; Hou, Y., *J. Phys. Chem. C* **2017**, *121*, 5154-5160.
19. Theoretical Study of Ripening Mechanisms of Pd Clusters on Ceria. Su, Y.-Q.; ***Liu, J.-X.***; Filot, I. A. W.; Hensen, E. J. M., *Chem. Mater.* **2017**, *29*, 9456-9462.
18. Stable Pd-Doped Ceria Structures for CH_4 Activation and CO Oxidation. Su, Y.-Q.; Filot, I. A.; ***Liu, J.-X.***; Hensen, E. J., *ACS Catal.* **2017**.
17. First-Principles Study of Structure Sensitivity of Chain Growth and Selectivity in Fischer–Tropsch Synthesis Using Hcp Cobalt Catalysts. Su, H.-Y.; Zhao, Y.; ***Liu, J.-X.***; Sun, K.; Li, W.-X., *Catal. Sci. Technol.* **2017**.
16. Particle Size and Crystal Phase Effects in Fischer-Tropsch Catalysts. ***Liu, J.-X.***; Wang, P.; Xu, W.; Hensen, E. J. M., *Engineering* **2017**, *3*, 467-476.
15. CO Oxidation on Rh-Doped Hexadecagold Clusters. ***Liu, J.-X.#***; Liu, Z.#; Filot, I. A.; Su, Y.; Tranca, I.; Hensen, E. J., *Catal. Sci. Technol.* **2017**, *7*, 75-83.
14. Chemical Insights into the Design and Development of Face-Centered Cubic Ruthenium Catalysts for Fischer–Tropsch Synthesis. Li, W.-Z.#; ***Liu, J.-X.#***; Gu, J.#; Zhou, W.; Yao, S.-Y.; Si, R.; Guo, Y.; Su, H.-Y.; Yan, C.-H.; Li, W.-X.; Zhang, Y.-W.; Ma, D., *J. Am. Chem. Soc.* **2017**, *139*, 2267.
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11. Theoretical Study of Crystal Phase Effect in Heterogeneous Catalysis. ***Liu, J. X.***; Li, W. X., *WIREs: Comput. Mol. Sci.* **2016**, *6*, 571-583.
10. High Alcohols Synthesis Via Fischer–Tropsch Reaction at Cobalt Metal/Carbide Interface. Pei, Y.-P.#; ***Liu, J.-X.#***; Zhao, Y.-H.; Ding, Y.-J.; Liu, T.; Dong, W.-D.; Zhu, H.-J.; Su, H.-Y.; Yan, L.; Li, J.-L.; Li, W.-X., *ACS Catal.* **2015**, *5*, 3620-3624.
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8. A First-Principles Study of Carbon–Oxygen Bond Scission in Multiatomic Molecules on Flat and Stepped Metal Surfaces. Zhao, Y.-H.; ***Liu, J.-X.***; Su, H.-Y.; Sun, K.; Li, W.-X., *ChemCatChem* **2014**, *6*, 1755-1762.
7. Co–Co_2C and Co–Co_2C/Ac Catalysts for Hydroformylation of 1-Hexene under Low Pressure: Experimental and Theoretical Studies. Dong, W.#; ***Liu, J.-X.#***; Zhu, H.; Ding, Y.; Pei, Y.; Liu, J.; Du, H.; Jiang, M.; Liu, T.; Su, H.; Li, W., *J. Phys. Chem. C* **2014**, *118*, 19114-19122.
6. Platinum-Modulated Cobalt Nanocatalysts for Low-Temperature Aqueous-Phase Fischer–Tropsch Synthesis. Wang, H.#; Zhou, W.#; ***Liu, J.-X.#***; Si, R.; Sun, G.; Zhong, M.-Q.; Su, H.-Y.; Zhao, H.-B.; Rodriguez, J. A.; Pennycook, S. J.; Idrobo, J.-C.; Li, W.-X.; Kou, Y.; Ma, D., *J. Am. Chem. Soc.* **2013**, *135*, 4149-4158.
5. Atomistic Theory of Ostwald Ripening and Disintegration of Supported Metal Particles under Reaction Conditions. Ouyang, R.; ***Liu, J.-X.***; Li, W.-X., *J. Am. Chem. Soc.* **2013**, *135*, 1760-1771.
4. Crystallographic Dependence of CO Activation on Cobalt Catalysts: Hcp Versus Fcc. ***Liu, J.-X.#***; Su, H.-Y.#; Sun, D.-P.; Zhang, B.-Y.; Li, W.-X., *J. Am. Chem. Soc.* **2013**, *135*, 16284-16287.
3. Structure Sensitivity of CO Methanation on Co (0001), (10-12) and (11-20) Surfaces: Density Functional Theory Calculations. Liu, J.-X.; Su, H.-Y.; Li, W.-X., *Catal. Today* **2013**, *215*, 36-42.
2. Structural and Electronic Properties of Cobalt Carbide Co_2C and Its Surface Stability: Density Functional Theory Study. Zhao, Y.-H.; Su, H.-Y.; Sun, K.; ***Liu, J.***; Li, W.-X., *Surf. Sci.* **2012**, *606*, 598-604.
1. Carbon Chain Growth by Formyl Insertion on Rhodium and Cobalt Catalysts in Syngas Conversion. Zhao, Y.-H.; Sun, K.; Ma, X.; ***Liu, J.***; Sun, D.; Su, H.-Y.; Li, W.-X., *Angew. Chem. Int. Ed.* **2011**, *50*, 5335-5338.

(INVITED) PRESENTATIONS

10. ***Jin-Xun Liu,*** Identifying the active structures of metal nanoparticles supported on CeO2 for CO oxidation, 257th ACS national meeting, 2019.3, Orlando, USA
9. ***Jin-Xun Liu,*** Identification of active structure of CeO2 supported transition metal nanoparticles, The 4th computational catalysis symposium, 2019.4, Xi'an, China
8. ***Jin-Xun Liu,*** Activity and Selectivity Trends in Electrocatalytic Nitrate Reduction on Transition Metals, NAM 26. 2019 North American Catalysis Society Meeting, 2019.6, Chicago, USA
7. ***Jin-Xun Liu***, The catalytic activity of heterogeneous catalysis, invitation talk, National Chemistry Conference, 2018.5, China

6. ***Jin-Xun Liu***, Emiel J.M. Hensen, A novel strategy to identify the active phase structure of heterogeneous catalysts, oral, The Netherlands' Catalysis and Chemistry Conference. 2018.3, Netherlands.
5. ***Jin-Xun Liu***, Emiel J.M. Hensen, Gold particle size effect for CO oxidation, oral, The Netherlands' Catalysis and Chemistry Conference. 2017.3, Netherlands.
4. ***Jin-Xun Liu***, Emiel J.M. Hensen, New Tetrahedral Gold-Cage Nanocluster for CO oxidation: DFT calculation study. Poster, 16th international conference on catalysis, Beijing, China, 2016.7
3. ***Jin-Xun Liu***, Emiel J.M. Hensen, CO oxidation on Rh-doped Au_{16} cluster. Poster, Chains conference in Netherlands. 2015.12, Netherlands
2. ***Jin-Xun Liu***, Hai-Yan Su, Bing-Yan Zhang and Wei-Xue Li, Crystallographic Dependence of CO Activation on Cobalt Catalysts: HCP versus FCC, The 12th national conference of quantum chemistry, Poster, 2014, Taiyuan, China
1. ***Jin-Xun Liu***, Hai-Yan Su and Wei-Xue Li, Structure Sensitivity of CO Methanation on Cobalt (0001), (10-12) and (11-20) Surfaces: Density Functional Theory Calculations, The 16th national congress on catalysis, Poster, 2012, Shenyang, China

PROFESSIONAL SERVICE AND EDUCATIONAL ACTIVITIES

Refereed papers in journals such as: *Iscience, ACS Catal., Chem. Comm., J. Phys. Chem. C, J. Mater. Chem. A, Chem. Engin. Sci., Appl. Surf. Sci., Catal. Sci. Technol., Chem. Eng. Sci., ACS Appl. Mater. and so on.*