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EDUCATION

Peking University, Beijing, Doctor of Natural Science (Physical Chemistry), July 2016

Peking University, Beijing, Bachelor of Science (Chemistry), July 2011

RESEARCH INTERESTS

Multiscale Simulations of Surface Chemical Reactions

ab initio Molecular Dynamics Simulation

Structure Prediction

Physical Chemistry of Surfaces and Interfaces by First-Principles Calculations

Machine Learning for Data Analysis

PUBLICATIONS

Journal Article

Geng Sun, Hong Jiang, "Ab initio molecular dynamics with enhanced sampling for surface reaction kinetics at finite temperatures: $CH_2 \rightleftharpoons CH + H$ on Ni(111) as a Example", THE JOURNAL OF CHEMICAL PHYSICS, 2015, 143, 234706.

Peng Zhai, Geng Sun, Qingjun Zhu, Ding Ma, "Fischer-Tropsch synthesis nanostructured catalysts: understanding structural characteristics and catalytic reaction", NANOTECHNOLOGY REVIEWS, 2013, 2, 547.

Hang Wang, Wu Zhou, Jinxun Liu, Rui Si, Geng Sun, Mengqi Zhong, Haiyan Su, Huabo Zhao, Jose A. Rodriguez, Stephen J. Pennycook, Juan-Carlos Idrobo, Weixue Li, Yuan Kou, Ding Ma, "Platinum-Modulated Cobalt Nanocatalysts for Low-Temperature Aqueous-Phase Fischer-Tropsch Synthesis", JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 2013, 135, 4149.

Jinghe Yang, Geng Sun, Yongjun Gao, Huabo Zhao, Pei Tang, Juan Tan, An-Hui Lu, Ding Ma, "Direct catalytic oxidation of benzene to phenol over metal-free graphene-based catalyst", ENERGY & ENVIRONMENTAL SCIENCE, 2013, 6, 793.

Xiao Yuan, Geng Sun, Hiroyuki Asakura, Tsunehiro Tanaka, Xi Chen, Yuan Yuan, Gabor Laurenczy, Yuan Kou, Paul J. Dyson, Ning Yan, "Development of Palladium Surface-Enriched

Heteronuclear Au–Pd Nanoparticle Dehalogenation Catalysts in an Ionic Liquid, CHEMISTRY-A EUROPEAN JOURNAL, 2013, 19, 1227.

Lingtao Liu, Geng Sun, Chen Wang, Jinghe Yang, Chaoxian Xiao, Hang Wang, Ding Ma, Yuan Kou, "Aqueous phase Fischer–Tropsch synthesis in a continuous flow reactor", CATALYSIS TODAY, 2012, 183, 136.

Conference Poster

Geng Sun, Hong Jiang, "DFT Study of Single Metal Atom Adsorption on $\alpha\text{-Al}_2\text{O}_3(0001)$ and Its Effects on Oxygen Vacancy Formation", The 15th International Congress of Quantum Chemistry, Beijing, 2015.

Geng Sun, Hong Jiang, "Study of Surface Structure by Integrated Tempering Sampling Method", 12th National Conference of Quantum Chemistry, Taiyuan, Shanxi, 2014.