



Department: School of Chemical Engineering

Professional field: Chemical engineering and technology

E-mail: yanzhu@ecust.edu.cn

Profile

Ph.D. in Chemical Engineering, 9/2002-6/2007

East China University of Science and Technology, China

Visiting Scholar, 8/2008-2/2009

Norwegian University of Science and Technology (NTNU), Norway;

Associate Professor, 9/2009-8/2016

East China University of Science and Technology, China;

Visiting Scholar, 1/2013-1/2014

Stanford University (SLAC National Accelerator Laboratory), the United States;

Professor, 9/2016-

East China University of Science and Technology, China

Research Field

1. Heterogeneous catalysis from first-principles calculations and microkinetic modeling

Studies on catalytic processes over metal and metal oxide surfaces through density functional theory (DFT) calculations to design new catalysts with high catalytic activity and selectivity; using the DFT-derived kinetic parameters for the elementary steps to examine the reaction mechanisms for the overall catalytic reactions within the framework of the microkinetics of heterogeneous catalysis

2. Molecular mechanics calculations based on force fields

Studies on the chemical and physical properties of new carbon materials through molecular mechanics calculations based on force fields; investigating the topological structures of new carbon materials on the microscopic scale using XRD simulations

Research results and selected published papers

1. Jun Zhu, Ming-Lei Yang, Ying-Da Yu, Yi-An Zhu*, Zhi-Jun Sui, Xing-Gui Zhou, Anders Holmen, De Chen*. Size-dependent reaction mechanism and kinetics for propane dehydrogenation over Pt catalysts. *ACS Catalysis*, 2015, 5: 6310-9.
2. Ming-Lei Yang, Chen Fan, Yi-An Zhu*, Zhi-Jun Sui, Xing-Gui Zhou, De Chen. Selective oxidation of hydrogen in the presence of propylene over Pt-based core-shell nanocatalysts. *The Journal of Physical Chemistry C*, 2015, 119(37): 21386-94.
3. Hong-Ye Cheng, Yi-An Zhu*, De Chen, Per-Olof Åstrand, Ping Li, Zhi-Wen Qi, Xing-Gui Zhou. Evolution of carbon nanofiber-supported Pt nanoparticles of different particle sizes: A molecular dynamics study. *The Journal of Physical Chemistry C*, 2014, 118(41): 23711-22.
4. Hong-Ye Cheng, Yi-An Zhu*, Zhi-Jun Sui, Xing-Gui Zhou, De Chen. Modeling of fishbone-type carbon nanofibers with cone-helix structures. *Carbon*, 2012, 50(12): 4359-72.
5. Chen Fan, Yi-An Zhu*, Yue Xu, Yan Zhou, Xing-Gui Zhou, De Chen. Origin of synergistic effect over Ni-based bimetallic surfaces: A density functional theory study. *The Journal of Chemical Physics*, 2012, 137(1): 014703.
6. Ming-Lei Yang, Yi-An Zhu*, Xing-Gui Zhou, Zhi-Jun Sui, De Chen*. First-principles calculations of propane dehydrogenation over PtSn catalysts. *ACS Catalysis*, 2012, 2(6): 1247-58.
7. Chen Fan, Xing-Gui Zhou, De Chen, Hong-Ye Cheng, Yi-An Zhu*. Towards CH₄ dissociation and C diffusion during Ni/Fe-catalyzed carbon nanofiber growth: A density functional theory study. *The Journal of Chemical Physics*, 2011, 134(13): 134704.
8. Yi-An Zhu*, Xing-Gui Zhou*, De Chen, Wei-Kang Yuan. First-principles study of C adsorption and diffusion on the surfaces and in the subsurfaces of nonreconstructed and reconstructed Ni(100). *The Journal of Physical Chemistry C*, 2007, 111(8): 3447-53.
9. Yi-An Zhu*, Ying-Chun Dai, De Chen, Wei-Kang Yuan*. First-principles study of carbon diffusion in bulk nickel during the growth of fishbone-type carbon nanofibers. *Carbon*, 2007, 45(1): 21-7.
10. Yi-An Zhu, Zhi-Jun Sui, Tie-Jun Zhao, Ying-Chun Dai, Zhen-Min Cheng, Wei-Kang Yuan*. Modeling of fishbone-type carbon nanofibers: A theoretical study. *Carbon*, 2005, 43(8): 1694-9.