



所属学院 化工学院

学科领域 化学工程与技术

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个人简介

2002/09 - 2007/06, 华东理工大学, 化工学院, 博士
2008/08 - 2009/02, 挪威科技大学, 化工系, 访问学者
2009/09 - 2010/03, 华东理工大学, 化工学院, 副研究员
2013/01 - 2014/01, 美国斯坦福大学, 化工系, SLAC 国家实验室, 访问学者
2016/09 - 至今, 华东理工大学, 化工学院, 教授

研究方向

1. 多相催化与化学反应工程。主要研究包含丙烷脱氢、甲烷蒸汽（干气）重整、甲烷部分氧化、乙烯选择性加氢、苯部分加氢和乙苯脱氢等化学工业中涉及的或者具有工业化前景的反应过程动力学；
2. 基于表面化学的微观动力学研究。通过密度泛函理论计算，在统计热力学和过渡态理论框架下获取反应机理，并依据火山形曲线进行高通量催化剂筛选；
3. 基于新型纳米炭材料的催化剂（载体）研究。主要包含纳米碳纤维、碳纳米管等新型材料的结构化学研究，并以可调变结构的炭材料为催化剂载体平台，研究载体结构调变活性金属催化性能的普遍规律。

研究成果及主要发表文章

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.