化学系 | Department Of Chemistry

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韩波，湖北仙桃人，1982年7月出生，2005年毕业于中国地质大学(武汉)应用化学专业，2010年在中国地质大学(武汉)获博士学位，2011.9-2012.9期间在新加坡国立大学化学系作博士后研究。主要从事计算化学与计算材料学方面的研究工作。研究领域涉及表面化学、能源材料、均相与多相催化等方面。已发表SCI论文20余篇(点击查看)，发布美国专利2项、欧洲专利1项、日本专利1项。

教育背景(Education)

学位	起止时间	学校与学院	专业
学士	2001.9-2005.6	中国地质大学(武汉)材料与化学学院	应用化学
硕士	2005.9-2008.6	中国地质大学(武汉)材料与化学学院	应用化学
博士	2008.9-2010.12	中国地质大学(武汉)材料与化学学院	岩石矿物材料学

工作经历(Work Experiences)

起止时间	工作单位	职位
2011.3-	中国地质大学(武汉)材料与化学学院	教师
2011.9-2012.9	新加坡国立大学化学系	博士后

研究领域(Research Interests)

1. 表面化学：1). 半导体表面功能薄膜的沉积行为和机理; 2). 异相/均相催化反应行为及先进催化剂的设计。
   Surface Chemistry: 1). Deposition behaviors and mechanisms of functional films on semiconductor surfaces; 2). Developing homogeneous/heterogeneous catalysts and investigating the catalytic behaviour.
2. 电化学：1). 新型电极材料的研发; 2). 电化学过程的界面行为。
   Electrochemistry: 1). Developing novel materials for electrode; 2). Interfacial behavior during electrochemic process.

招生倾向 (Student Preferences)

1. 具有较好的结构化学基础知识;
2. 或具有较好的电化学基础知识;

3. 或具有较好的有机合成功底和经验.

项目列表 (Funds)

1. 《二氧化硅薄膜的原子层沉积反应机理及前驱体设计》, 国家自然科学基金青年项目
项目经费24.0万元, 2013.1-2015.12, 主持；
2. 《新型原子层沉积前驱体的计算、设计与制备》, 中央高校基本科研业务费专项资金资助项目
项目经费5.0万元, 2011.11-2013.12, 主持；
3. 《石墨烯/氧化物半导体复合体系在光伏转换与光催化制氢/氢解耦合反应中的应用》， 中国地质大学(武汉)中央高校第二批
色学科团队
项目经费100.0万元, 2012.6-2015.5, 团队成员；
4. 《纳米粒子反应立场方法发展及其分子动力学模拟软件的实现》, 中国地质大学(武汉)"腾飞计划"人才基金
项目经费30.0万元, 2011.6-2014.5, 排名第二；
5. 《Pt,Pd,Ni团簇和纳米颗粒催化氢反应力场的建立》, 国家自然科学基金面上项目
项目经费32.0万元, 2010.1-2012.12, 排名第三 (项目编号 20973159)；
6. 《半导体芯片中Cu互联线廉价胶水材料的原子层沉积前驱体分子设计与制备》, 国家自然科学基金面上项目
项目经费28.0万元, 2009.1-2011.12, 排名第三 (项目编号20873127)
7. 《Computational Screening of Sillicon Nitride Precursors for Low Temperature Deposition》等，国际合作项目
项目经费34.5万美元, 2005.9-2012.12，排名第三 (项目编号201-828-P)

论文(Publications)

21. **Bo Han**, Yubao Sun, Maohong Fan, Hansong Cheng*, “On the CO2 Capture in Water-Free Monoethanolamine Solution: An ab In Molecular Dynamics Study”. *J. Phys. Chem. B*, 117:5971-5977 (2013). 【IF= 3.607】 DOI: 10.1021/jp4022932
20. Huang Liang, **Bo Han***, Bin Han, A. Derecskei-Kovacs, M. Xiao, X. Lei, M. L. O’Neill, R. M. Pearlstein, H. Chan Hansong Cheng*, “First-Principles Study of a Full Cycle of Atomic Layer Deposition of SiO2 Thin Films with Di(sec-butylamino)sil and Ozone”. *J. Phys. Chem. C*, 117:19454-19463 (2013). 【IF= 4.805】 DOI: 10.1021/jp405541x
19. Gang Ni, **Bo Han***, Hansong Cheng*, “Effect of Al Electronic Configuration on the SiO2 Thin Film Growth Catalytic Self-Assembling Deposition”. *J. Phys. Chem. C*, 117:22705-22713 (2013). 【IF= 4.80 DOI: 10.1021/jp405847r
18. **Bo Han**, Qingfan Zhang, Jinping Wu, Bing Han, Eugene J. Karwacki, Agnes Derecskei, Manchao Xiao, Xinjian Lei, Mark L. O’N Hansong Cheng*, “On the Mechanisms of SiO2 Thin-Film Growth by the Full Atomic Layer Deposition Process Using (t-butylamino)silane on the Hydroxylated SiO2(001) Surface”, *J. Phys. Chem. C*, 116:947-952 (2012). 【IF= 4.805】 DOI: 10.1021/jp2094802
17. Ming Yang, **Bo Han***, Hansong Cheng*, “First-Principles Study of Hydrogenation of Ethylene on a HxMoO3(0 Surface”. *J. Phys. Chem. C*, 116:24630-24638 (2012). 【IF= 4.805】 DOI: 10.1021/jp308255a
16. Qinfan Zhang, **Bo Han**, Xiaowei Tang, Kevin Heier, Jimmy X. Li, John Hoffman, Minfa Lin, Stephanie L. Brit Agnes Derecskei-Kovacs, Hansong Cheng*, “On the Mechanisms of Carbon Formation Reaction on Ni(111) Surface”, *J. Phys. Chem. C* 116:16522-16531 (2012) DOI: 10.1021/jp303648c
15. **Bo Han**, Chenggang Zhou, Jinping Wu, D. J. Tempel, Hansong Cheng*, “Understanding CO2 Capture Mechanisms in Aque Monoethanolamine via First Principles Simulations”. *J. Phys. Chem. Lett.*, 2:522-526 (2011). 【I 6.585】 DOI: 10.1021/jz200037s
14. Qinfan Zhang, **Bo Han**, Kevin Heier, Jimmy X. Li, John Hoffman, Minfa Lin, Agnes Derecskei-Kovacs, Hans Cheng*, “First Principles Study of Steam Carbon Reaction on γ-Fe(111) Surface”, *J. Phys. Chem. C* 115:12068-12 (2011) DOI: 10.1021/jp2019507
13. Lei Chen, Gang Ni, **Bo Han**, Chenggang Zhou, Jinping Wu*, “Mechanism of Water Gas Shift Reaction on Fe3 (111) Surface”. *Acta Chim. Sinica*, 69:393-398 (2011). full text
12. **Bo Han**, Jinping Wu*, Chenggang Zhou, Bei Chen, Roy Gordon, Xinjian Lei, David A. Roberts, Hansong Cheng*, “First-princi Simulations of Conditions of Enhanced Adhesion Between Copper and TaN(111) Surfaces Using a Variety of Metallic Glue Material *Angew. Chem. Int. Ed.*, 49:148-152 (2010). 【IF= 13.734】 DOI: 10.1002/anie.200905360
11. Chenggang Zhou, Qingfan Zhang, Lei Chen, **Bo Han**, Gang Ni, Jinping Wu, Diwakar Garg, Hansong Cher “Density Functional Theory Study of Water Dissociative Chemisorption on the Fe3O4(111) Surface”, *J. Phys. Ch C*, 114:21405-21410 (2010). DOI: 10.1021/jp105040v
10. Lei Chen, Qinfan Zhang, Yunfeng Zhang, Winston Z. Li, **Bo Han**, Chenggang Zhou, Jinping Wu*, Robert C. For Diwakar Garg, Hansong Cheng*, “A first principles study of water dissociation on small copper clusters”, *P Chem. Chem. Phys.*, 12:9845-9851 (2010). DOI: 10.1039/c001006e
9. Bei Chen, **Bo Han**, Chenggang Zhou, Jinping Wu*, “A Molecular Dynamic Simulation on the Agglomera Behavior of Cu on TaN(111) surface”. *Earth Science*, 34:635-640 (2009). full text
8. Shujuan Yao, Chenggang Zhou, **Bo Han**, Ting Fan, Jinping Wu, Liang Chen, Hansong Cheng*. “Chemisorptio small fullerenes Cn (n=28,32,36,40,44,48,60) on the Si(001)-c(2x1) surface”. *Phys. Rev. B*, 79:155304 (2009). DOI 10.1103/PhysRevB.79.155304
7. Jiaye Li, Jinping Wu, Chenggang Zhou, **Bo Han**, Xinjian Lei, Roy Gordon, Hansong Cheng*. “On the rela stability of cobalt- and nickel-based amidinate complexes against beta-migration”. *Int. J. Quantum Chem.* 109: 7 763 (2009). DOI: 10.1002/qua.21880
6.

Bo Han, Jinping Wu*, Chenggang Zhou, Jiaye Li, Xinjian Lei, John A. T. Norman, Thomas R. Gaffney, Roy Gordon, David A. Robe Hansong Cheng*. “Ab Initio Molecular Dynamics Simulation on the Aggregation of a Cu Monolayer on a WN(001) Surface”. *J. Phys. Chem. C*, 112:9798-9802 (2008). 【**IF= 4.805**】 DOI: 10.1021/jp802979b

5. Chenggang Zhou, Shujuan Yao, **Bo Han**, Liang Chen, Jinping Wu, Robert R. Forrey, and Hansong Cheng*, Mechanistic Study of CO Removal on a Small H-Saturated Platinum Cluster”, *Science in China, Series B: Chemis* 51:1187-1196 (2008). DOI: 10.1007/s11426-008-0135-z
4. Shujuan Yao, Chenggang Zhou, Jinping Wu, Jiaye Li, **Bo Han**, Hansong Cheng*, “On the electronic structures spectroscopic properties of polyyne and its derivatives”. *Int. J. Quantum Chem.*, 108:1565-1571 (2008). DOI: 10.1002/qua.21697
3. Jiaye Li, Jinping Wu, Chenggang Zhou, Shujuan Yao, **Bo Han**, “Influence of Nitrogen Substituent of Amidi Ligands to the Stability of Co(II) bis-amidinate ALD Precursors”. *Acta Chim. Sinica*, 66:165-169 (2008). full text
2. Jinping Wu, **Bo Han**, Chenggang Zhou, Xinjian Lei, T. R. Gaffney, John A. T. Norman, Zhengwen Li, Roy Gorc Hansong Cheng*. “Density Function Theory Study of Copper Agglomeration on the WN(001) Surface”. *J. P Chem. C*, 111:9403-9406 (2007). DOI: 10.1021/jp072907q
1. Chenggang Zhou, Jinping Wu, **Bo Han**, Shujuan Yao, Hansong Cheng*. “Adsorption of fullerenes (n=32,36,40,44,48,60) on the GaAs(001)-c(4x4) reconstructed surface”. *Phys. Rev. B*, 73:195324 (2006). DOI: 10.1103/PhysRevB.73.195324

国际专利**(International Patents)**

1. Cheng H, Lei X, Spence D, Norman J, Robert D, Han B, Zhou C, Wu J. "Method for Suppressing Agglomeration and Improving Semiconductor Device Adhesiveness". **Japanese Patent** JP2010062555. Application Number: JP2009000188053.
2. Cheng H, Lei X, Spence D, Norman J, Robert D, Han B, Zhou C, Wu J. "Materials for adhesion enhancement of copper film on diffus barriers". **European Patent Application** EP2154717. Application Number: EP20090167949.
3. Cheng H, Lei X, Spence D, Norman J, Robert D, Han B, Zhou C, Wu J. "Materials for Adhesion Enhancement of Copper Film on Diffusion Barriers". **US patent** US7919409. Application Number: 12/192603.
4. Cheng H, Lei X, Spence D, Norman J, Robert D, Han B, Zhou C, Wu J. "Materials for Adhesion Enhancement of Copper Film on Diffusion Barriers". **US patent application** US20100038785. Application Number: 12/192603.