

1.A highly active and stable Fe-Mn catalyst for slurry Fischer-Tropsch synthesis, Yong Yang, Hongwei Xiang, Rongle Zhang, Bing Zhong and Yongwang Li, *Catalysis Today*, 2005,106(1-4):170-175

2.An environmentally benign route to γ -butyrolactone through the coupling of hydrogenation and dehydrogenation, Yu-Lei Zhu, Jun Yang, Gen-Quan Dong, Hong-Yan Zheng, Hao-Hong Zhang, Hong-Wei Xiang, Yong-Wang Li, *Appl. Catal. B*, 2005,57(3):183-190

3.An ONIOM study of amines adsorption in H-[Ga]MOR, Jiang N; Yuan S P; Wang J G; Qin Z F; Jaio H J; Li Y W, *J. Mol. Catal. A*, 2005,232(1-2):59-67

4.Chemisorption of CO₂ on nickel surfaces, Sheng-Guang Wang, Dong-Bo Cao, Yong-Wang Li, Jianguo Wang,, Haijun Jiao, *J. Phy. Chem. B*, 2005,109(40):18956-18963

5.Density functional theory study of CO adsorption on molybdenum sulfide, Tao Zeng, Xiao-Dong Wen, Gui-Sheng Wu, Yong-Wang Li, Haijun Jiao; *J. Phys. Chem. B*. 2005,109(7); 2846-2854.

6.Density functional Theory Study of Hydrogen Adsorption on Fe₅C₂(001), Fe₅C₂(110), and Fe₅C₂(100), Dong-Bo Cao, Fu-Qiang Zhang, Yong-Wang Li, Jianguo Wang, and Haijun Jiao, *J. Phys. Chem. B*, 2005,109(2), 833-844

7.Density functional theory study of triangular molybdenum sulfide nanocluster and CO adsorption on it, Tao Zeng, Xiao-Dong Wen, Yong-Wang Li, and Haijun Jiao, *J. Phy. Chem. B*, 2005,109(28):13704-13710

8.Effect of air-exposure on reduction behavior of a Fe–Mn–Cu–K/SiO₂ Fischer-Tropsch synthesis catalyst, Chenghua Zhang, Botao Teng, Yong Yang, Zhichao Tao, Qinglan Hao, Haijun Wan, Fan Yi, Binfu Xu, Hongwei Xiang and Yongwang Li, *J. Mol. Catal. A*, 2005,239(1-2): 15-21

9.Effect of reduction temperature and duration on iron-based catalysts for slurry phase Fischer-Tropsch synthesis, Hao Qing-lan, Bai Liang, Hao Xu, Xiang Hong-wei, Li Yongwang, Yi Fan, Xu Bin-fu, 燃料化学学报, 2005,33(5):590-596

10. Effect of ZrO₂ promoter on structural change of Co/SiO₂ catalyst during its deactivation in F-T synthesis, Chang Jie, Chen Jiangang, Teng Botao, Xiang Hongwei, Li Yongwang, Sun Yuhan, Liu Tao, Xie Yaning, Zhang Jing, Hu Tiandou, 催化学报, 2005, 26(9):731-733

11. Formation of oxygen vacancies on the TiO₂(110) surfaces, Sheng-Guang Wang , Xiao-Dong Wen , Dong-Bo Cao, Yong-Wang Li ,Jianguo Wang, Haijun Jiao, Surf. Sci., 2005, 577(1), 69-76

12. Hydroformylation and isomerization of allene and propyne: a density functional theory study, Chun-Fang Huo, Yong-Wang Li, Matthias Beller, Haijun Jiao, Chem. Eur. J., 2005, 11(3); 889-902

13. Insight into the structure and intrinsic stability of the Keggin and Wells-Dawson neutral cages, Fu-Qiang Zhang, Hai-Shun Wu, Dong-Bo Cao, Xian-Ming Zhang, Yong-Wang Li, Haijun Jiao, J. Mol. Structure-Theochem, 2005, 755(1-3):119-126

14. Mechanism of thiophene hydrodesulfurization on a Mo₃S₉ model catalyst. A computational study, Xiao-Qian Yao, Yong-Wang Li, Haijun Jiao, J. Mol. Struct.(Theochem), 2005, 726(1-3):81-92

15. Mechanistic aspects of catalyzed benzothiophene hydrodesulfurization. A density functional theory study, Xiao-Qian Yao, Yong-Wang Li, Haijun Jiao, J. Mol. Struct.(Theochem), 2005, 726(1-3):67-80

16. Novel precipitated iron Fischer-Tropsch catalysts with Fe₃O₄ coexisting with-Fe₂O₃, Baoshan Wu, Lei Tan, Hongwei Xiang, Zhixin zhang, Yong-wang Li, Catal. Lett., 2005, 102(3-4):211-218

17. On the alpha/beta-[AlW₁₂O₄₀](5-) stability: Revisited, Fu-Qiang Zhang, Hai-Shun Wu, Xiao-Fang Qin, Yong-Wang Li, Haijun Jiao, J. Mol. Structure-Theochem 2005, 755(1-3):113-117

18. Oxygenate kinetics in Fischer-Tropsch synthesis over an industrial Fe–Mn catalyst, Bo-Tao Teng, Cheng-Hua Zhang, Jun Yang, Dong-Bo Cao, Jie Chang, Hong-Wei Xiang, Yong-Wang Li, Fuel, 2005, 84(7-8):791-800

19. Regioselective hydroformylation of butadiene: Density functional studies, Chun-Fang Huo, Yong-Wang

Li, Matthias Beller, Haijun Jiao, Organometallics, 2005,24(15):3634-3643

20. Removal of surface sulfur from MoSX cluster under CO adsorption, Tao Zeng, Xiao-Dong Wen , Yong-Wang Li , Haijun Jiao, J. Mol. Catal. A, 2005,241(1-2):219-226

21. Structure and Fischer-Tropsch performance of iron–manganese catalyst incorporated with SiO₂, Yong Yang, Hong-Wei Xiang, Lei Tian, Hong Wang, Cheng-Hua Zhang, Zhi-Chao Tao, Yuan-Yuan Xu, Bing Zhong and Yong-Wang Li, Appl. Catal. A, 2005,284(1-2):105-122

22. Structures and energies of coadsorbed CO and H₂ on Fe₅C₂(001)Fe₅C₂(110), and Fe₅C₂(100), Dong-Bo Cao, Fu-Qiang Zhang, Yong-Wang Li, Jianguo Wang, Haijun Jiao, J. Phy. Chem. B, 2005,109(21):10922-10935

23. Surface structure and energetics of hydrogen adsorption on the Fe(III)surface, Chun-Fang Huo, Yong-Wang Li, Jianguo Wang,Haijun Jiao (Reprint), J. Phy. Chem. B, 2005,109(29):14160-14167

24. Surface structure and energetics of oxygen and CO adsorption on alpha-Mo₂C(0001), Jun Ren, Chun-Fang Huo, Jianguo Wang, Yong-Wang Li, Haijun Jiao, Surface Science, 2005,596(1-3):212-221

25. Surface structure and stability of MoS_x model clusters, Xiao-Dong Wen, Tao Zeng, Yong-Wang Li, Jianguo Wang, Haijun Jiao (Reprint), J. Phy. Chem. B, 2005,109(39):18491-18499

26. Switching End-on into side-on C N coordination: A computational approach, Chun-Fang Huo, Tao Zeng, Yong-Wang Li, Matthias Beller, Haijun Jiao, Organometallics, 2005,24(24):6037-6042

27. Theoretical ONIOM2 study on pyridine adsorption in the channels and intersection of ZSM-5, Shuping Yuan, Wei Shi, Bingrui Li, Jianguo Wang, Haijun Jiao, Yong-Wang Li, J. Phy. Chem. A, 2005,109(11):2594-2601

28. Water gas shift reaction kinetics in Fischer–Tropsch synthesis over an industrial Fe–Mn catalyst, Bo-Tao Teng, Jie Chang, Jun Yang, Gang Wang, Cheng-Hua Zhang, Yuan-Yuan Xu, Hong-Wei Xiang, Yong-Wang Li, Fuel, 2005,84(7-8):917-926