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讲授课程情况	《物理化学》、《结构化学》、《科技外语》		
研究方向	利用基于密度泛函理论的第一性原理计算模拟及预测无机材料的物理性能		
	1. **Xianfeng Hao**, Yuanhui Xu, Zhijian Wu, Defeng Zhou, Xiaojuan Liu, Xueqiang Cao and Jian Meng, Low compressibility and hard materials ReB2 and WB2: prediction from first-principles study, **Phys. Rev. B** 74, 224112 (2006).（SCI 收录） 2. **Xianfeng Hao**, Zhijian Wu, Yuanhui Xu, Defeng Zhou, Xiaojuan Liu, and Jian Meng, Trends in elasticity and electronic structure of 5d transition metal diborides: first-principles calculations, **J. Phys.: Condens. Matter** 19,		

近三年发表文章情况	196212 (2006).SCI收录） 3.**Xianfeng Hao**, Yuanhui Xu, Zhijian Wu, Defeng Zhou, Xiaojuan Liu, and Jian Meng, Orbital ordering in Cs2AgF4: from first-principles DFT calculations, **Phys. Rev. B** 76, 054426 (2007). （SCI收录） 4.**Xianfeng Hao**, Yuanhui Xu, Zhijian Wu, Defeng Zhou, Xiaojuan Liu, and Jian Meng, Elastic anisotropy of OsB2 and RuB2 from first principles study, **J. Alloy & Comp.** 453, 413 (2008). （SCI收录） 5.**Xianfeng Hao**, Yuanhui Xu, Minfeng Lv, Defeng Zhou, Zhijian Wu, and Jian Meng, Charge, orbital, and magnetic ordering in YBaFe2O5 from first-principles calculations, **Inorg. Chem.** 47,4734 (2008).（SCI收录） 6*.**Xianfeng Hao**, Yuanhui Xu, Faming Gao, Defeng Zhou and Jian Meng, Charge disproportionation in CaCu3Fe4O12, **Phys. Rev. B** 79, 113101 (2009). （SCI收录） 7*.**Xianfeng Hao**, Yuanhui Xu and Faming Gao, Electronic and elastic properties of newsemiconducting oP12-type RuB2 and OsB2, **J. Phys.: Condens. Matter** 23 125501 (2011). （SCI收录） 8*.**Xianfeng Hao**, Yuanhui Xu, Zhiping Li, Lei Wang, Faming Gao and Debao Xiao, Elastic properties of novel Rhenium Nitrides from first principles, **Phys. Status Solidi b** (in press). （SCI收录） 9. Yuanhui Xu, **Xianfeng Hao**, Minfeng Lv, Zhijian Wu, Defeng Zhou and Jian. Meng, Magnetic structure and orbital ordering in tetragonal and monoclinic KCrF3 from first-principles calculations, **J. Chem. Phys.** 128, 164721(2008). （SCI收录） 10.Yuanhui Xu, **Xianfeng Hao**, Minfeng Lv, Zhijian Wu, Defeng Zhou and Jian. Meng, Electronic and magnetic properties of YBa2Fe3O8 from a first-principles study, **Solid State Commun.** 147,130 (2008). （SCI收录） 11.Zhijian Wu，**Xianfeng Hao**, Xiaojuan Liu, and Jian Meng, Structures and elastic properties of OsN2 investigated via first-principles density functional calculations, **Phys. Rev. B** 75, 054115(2007) （SCI收录） 12.Yuanhui Xu, **Xianfeng Hao**, Jian Meng, Defeng Zhou and Faming Gao，Electronic and magnetic properties of the monoclinic phase BiCrO3 from first-principles studies, **J. Phys.:Condens. Matter** 21, 236006 (2009). （SCI收录） 13.Yuanhui Xu, Faming Gao and **Xianfeng Hao**, Theoretical hardness and ideal tensile strength of bct-C4, **Phys. Status Solidi RRL** 4, 200 (2010). （SCI收录） 14.Yuanhui Xu, Faming Gao, **Xianfeng Hao**, Zhiping Li, Electronic structure and magnetism in superconductor ZnNNi3: A comparative study with ZnCNi3 and ZnNi3, **Comput. Mater. Sci.** 50,737 (2010). （SCI收录） 15.Zhijian Wu, Erjun Zhao, Hongping Xiang, **Xianfeng Hao**, Xiaojuan Liu and Jian Meng, Crystal structures and elastic properties of superhard IrN2 and IrN3 from first principles, **Phys.Rev. B** 76, 054115(2007). （SCI收录） * Corresponding author
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