

量子材料科学中心

International Center for Quantum Materials
Weekly Seminar

Unified model for spin order induced polarization in multiferroics



Hongjun Xiang

Key Laboratory of Computational Physical Sciences (Ministry of Education), State Key Laboratory of Surface Physics, and Department of Physics, Fudan University

- Time: 4:00pm, Oct. 23, 2013 (Wednesday)
- 时间: 2013年10月23日 (周三) 下午4:00
- Venue: Conference Room 607, Science Building 5
- 地点: 理科5号楼607

Abstract

In recent years, we have theoretically studied the microscopic origin of ferroelectricity in different multiferroic systems. We proposed a unified model [1,2] which includes purely electronic and ion-displacement contribution simultaneously to describe spin-order induced ferroelectricity. An efficient method [3] was developed to compute the model parameters from first-principles. On the basis of the unified model and density functional calculations, we explained the ferroelectricity induced by the proper-screw spin spiral [2], discovered a novel magnetoelectric coupling mechanism in which the magnitude of the polarization is governed by the exchange striction with the direction by the spin chirality [4], proposed that the ferroelectricity in the chiral-lattice magnet Cu_2OSeO_3 is due to the unusual single-spin site term [5], unraveled that the magnetoelectric effect observed in BiFeO_3 originates from the exchange striction [2].

References

- H. J. Xiang, E. J. Kan, Y. Zhang, M.-H. Whangbo, and X. G. Gong, *Phys. Rev. Lett.* **107**, 157202 (2011).
 H. J. Xiang, P. S. Wang, M.-H. Whangbo, and X. G. Gong, *Phys. Rev. B* **88**, 054404 (2013).
 H. J. Xiang, E. J. Kan, Su-Huai Wei, M.-H. Whangbo, and X. G. Gong, *Phys. Rev. B* **84**, 224429 (2011).
 X. Z. Lu, M.-H. Whangbo, Shuai Dong, X. G. Gong, and H. J. Xiang, *Phys. Rev. Lett.* **108**, 187204 (2012).
 J. H. Yang, Z. L. Li, X. Z. Lu, M.-H. Whangbo, Su-Huai Wei, X. G. Gong, and H. J. Xiang, *Phys. Rev. Lett.* **109**, 107203 (2012).

About the Speaker

向红军现为复旦大学物理系、应用表面物理重点实验室、物质计算科学教育部重点实验室教授。1997年9月至2006年7月就读于中国科学技术大学化学物理系，并获本科和博士学位。2006年9月至2009年底，分别在美国北卡州立大学和美国可再生能源国家实验室开展博士后研究。向红军长期从事计算凝聚态物理研究，主要开展计算方法的发展，结构和性质的预言和设计，模型计算等。特别地，在多铁性微观机制方面取得了进展：提出了自旋序诱导铁电性的普适性极化模型，并发展了相应的第一性原理计算方法；利用普适性极化模型解释了以前理论不能理解的多种复杂氧化物体系的多铁现象。其博士论文“纳米材料的理论研究及线性标度电子结构方法的发展”曾获2008年全国百篇优秀博士学位论文奖，2009年被授予上海高校特聘教授（东方学者）称号，2010年被评为教育部新世纪优秀人才。迄今发表SCI论文80多篇，其中Phys. Rev. Lett. 16篇。