



中心系列讲座 ICQM Weekly Seminar Series

“Electronic structures and magnetic orders of iron- pnictides or chalcogenides”



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Time: 4:00pm, Oct. 7, 2011 (Wednesday)

时间: 2011年10月19日 (周三) 下午4:00

Venue: Room 607, Conference Room A , Science Building 5

地点: 理科五号楼607会议室

Abstract

"The first-principles electronic structure calculations play an important role on study of high Tc superconductor iron- pnictides or chalcogenides. Iron-pnictides were first predicted by the theoretical calculations to be antiferromagnetic semimetals. Based on the calculations, Arsenic-bridged antiferromagnetic superexchange interaction was proposed. The bi-collinear antiferromagnetic order was then predicted for iron-chalcogenide α -FeTe. Recently, the parent compounds of superconductors iron-chalcogenides $KyFe(2-x)Se$ with ordered Fe vacancies were further shown to be antiferromagnetic semiconductors, in which the superconductivity emerges upon electron or hole doping, especially, the superconductivity and antiferromagnetic long-range order may coexist."

About the Speaker

卢仲毅于1996年在意大利国际高等研究院(SISSA)获得凝聚态物理学哲学博士学位。毕业后,先后在美国能源部Ames国家实验室、Vanderbilt大学物理系和Oak Ridge国家实验室计算机科学和数学部工作。2005年1月以中国科学院理论物理研究所百人计划聘为研究员和博士生导师。2007年1月聘为中国人民大学教授、物理系材料计算与物质模拟团队学科责任教授和召集人。主要从事电子结构计算方法及其并行化算法以及分子动力学模拟方法的研究以及这些方法在实际系统中的应用。