北京大学量子材料科学中心
International Center for Quantum Materials, PKU

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Electronic band structures of d- and f-electron systems from the GW@LDA+U perspective

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Venue: Room 607, Science Building 5
地点：理科五号楼607会议室

Abstract

The accurate first-principles description of d- and f-electron systems is currently regarded as one of the great challenges in condensed matter physics due to the simultaneous presence of itinerant (delocalized) and highly localized states and interactions between them. Density-functional theory (DFT) in the local-density approximation (LDA) proves to be inadequate for d/f-electron systems due to the severe self-interaction (delocalization) error. The simplest extension that can overcome the major failure of LDA is by introducing a local Hubbard like correction (LDA+U), which, however, treats itinerant states still at the LDA level. Many-body perturbation theory in the GW approach offers both a quasi-particle perspective (appropriate for itinerant states) and an exact treatment of exchange (appropriate for localized states). The combination of GW with LDA+U (GW@LDA+U) is therefore promising for d/f-electron systems. In this talk, I will present a systematic investigation of the GW@LDA+U approach, as implemented in our newly developed all-electron GW code FHI-GAP (Green's function with Augmented Planewaves) [1], for a series of prototypical d- and f-electron systems including later transition metal oxides [2], lanthanide oxides [3] and actinide oxides [4]. We observed good agreement between the GW density of states and experimental spectra using U determined by the constrained DFT approach. All main features found in experimental band gaps of the lanthanide sesquioxide series (Ln2O3) are well reproduced by our approach. Consistent with other GW approaches, the satellite structure in the photoemission spectroscopy of late transition metal oxides is still missing, and the binding energy of occupied d/f-states tends to be underestimated. We also compare GW@LDA+U to other variants of GW approaches as well as dynamical mean-field theory to illuminate pros and cons of different approaches. I will also present some recent work on first-principles determination of the Hubbard U in the constrained random phase approximation formalism.

[1] H. Jiang, R. Gomez-Abal, X. Li, H. Jiang, C. Meisenbichler, C. Ambrosch-Draxl, M. Scheffler, in preparation (2011).
[2] H. Jiang, R. Gomez-Abal, P. Rinke, and M. Scheffler, Phys. Rev. B 82, 045108 (2010)
[3] H. Jiang, R. Gomez-Abal, P. Rinke, and M. Scheffler, Phys. Rev. Lett. 102, 126403 (2009).
[4] H. Jiang, P. Rinke and M. Scheffler, in preparation (2011).

About the Speaker

蒋鸿，2003年北京大学化学与分子工程学院博士。先后在美国杜克大学，德国法兰克福大学，德国柏林Fritz-Haber研究所从事博士后研究工作。2008年12月作为“北大百人”特聘研究员进入北京大学化学与分子工程学院理论与计算化学研究所工作。主要研究方向是针对含过渡金属或镧系/锕系元素（d/f-电子）材料的理论方法发展与应用计算研究。