



TRR 80 Sonderseminar

Am Mittwoch, den 1. Februar um 15:00 Uhr

spricht

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über das Thema

Electronic and Magnetic Properties of Insulators with Correlated Electrons: ab initio Studies

For an adequate description of the electronic and magnetic ground state properties of correlated electron systems within density functional theory it is essential to go beyond standard approximations, such as LDA or GGA. One such possibility are the so-called self-interaction corrections (SIC) [1]. Using a local SIC implementation within a Greens Functions multiple scattering approach [2] allows, by applying a magnetic force theorem [3], for a calculation of the interaction parameters J of the Heisenberg model of magnetism. Knowing them provides information about properties such as the magnetic equilibrium structure, critical temperature and magnon dispersion.

In this talk, after introducing the method, results of investigations of several correlated electron systems are presented. They demonstrate that SIC significantly improves the agreement with experimental magnetic and electronic observables. The studied systems are transition metal monoxides [4] and fluorides, MnSe, and polar ZnO surfaces [5].

[1] Perdew, Zunger, PRB 23, 5048 (1981)

[2] Lüders et al., PRB 71, 205109 (2005) [3] Liechtenstein et al., JMMM 67,

65 (1987) [4] Däne et al., J. Phys.: Condens. Mat. 21, 045604 (2009);

Fischer et al., PRB 80, 014408 (2009) [5] Fischer et al., PRB 84, 205306 (2011)

Gäste sind herzlich willkommen.

Der Vortrag findet im Seminarraum S-403/ Institut für Physik, Universität Augsburg statt.

Gastgeber: Dr. Joachim Deisenhofer
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