Group Seminar: Magnetic Materials

Universität Konstanz

Prof. Dr. László Szunyogh
Budapest University of Technology and Economics

Do 04.11.21
13:30 Uhr
P712

Exchange interactions from a nonorthogonal basis set: Application to the magnetism of graphene systems

The ground state and thermal properties of magnetic systems, either characterized by itinerant electrons or by local moments, are most commonly described by a Hamiltonian parametrized in form of a spin model where, in the classical limit, the spins are allowed to fluctuate with their magnitude kept constant. For a given material the model parameters can be derived from first principles, in most cases relying on the magnetic force theorem as employed in the seminal work of Liechtenstein *et al*. [1].

In this talk I present a computational method for the direct evaluation of isotropic exchange interaction from density functional calculations using nonorthogonal basis sets. By giving some details of the derivation I show that the expression for the exchange interactions is formally identical with the one using orthogonal basis sets. We implemented the new method in the SIESTA code [2] and demonstrate that in case of simple metallic ferromagnets it adequately reproduces the Heisenberg interactions obtained from previous well established computational methods.

I report on the study of the magnetism of two systems based on graphene. For *fluorinated graphene* we obtained exchange constants in fairly good agreement with former calculations and we confirmed the theoretical prediction of a 120º Néel state. The long-range behavior of the exchange interactions was found consistent with the electron spectrum of the system around the Fermi level.

For *zigzag graphene nanoribbons* the stiffness constant derived from the exchange interactions was also consistent with previous estimates based on total energy differences of twisted spin confgurations. We, however, found an unconventional $\exp(-\sqrt{\Upsilon}/\delta)$-like decay of the interactions [3]. The described scheme holds a great promise for investigating novel two-dimensional magnets often displaying exotic magnetic patterns.

[1] A. I. Lichtenstein, M. I. Katsnelson, V. P. Antropov, and V. A. Gubanov, Journal of Magnetism and Magnetic Materials **67**, 65 (1987).

[2] https://departments.icmab.es/leem/siesta/

[3] L. Oroszlány, J. Ferrer, A. Deák, L. Udvardi, and L. Szunyogh, Physical Review B **99**, 224412 (2019).