On-line SPICE-SPIN+X Seminars

Wednesday, 19th January 2022, 15:00 (CET)

The seminar will be via Zoom (Meeting ID: 857 1369 9839**) and live streamed in the SPICE YouTube Channel.**

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Theory of magnetic interactions in real materials

Magnetic ordering and related phenomena are of essentially quantum and essentially many-body origin and require strong enough electron-electron interactions. Also, they are very sensitive to the details of electronic structure of specific materials. This makes a truly microscopic description of exchange interactions a challenging task. Long ago we suggested a general scheme of calculations of exchange interactions responsible for magnetism based on the "magnetic force theorem". It was formulated originally as a method to map the spin-density functional to effective classical Heisenberg model, the exchange parameters turned out to be, in general, essentially dependent on initial magnetic configuration and not universal. However, they are directly related to the spin-wave spectrum and, thus, can be verified experimentally. This approach also lies in the base of "ab initio spin dynamics" within the density functional approach. It is well known now that this scheme is, in general, insufficient for strongly correlated systems and should be combined with the mapping to the multiband Hubbard model and use of, say, dynamical mean-field theory (DMFT) to treat the latter. Our original approach can be reformulated within the DMFT.

The method can be also modified to calculate Dzialoshinskii-Moriya interactions which play a crucial role in the phenomenon of weak ferromagnetism, in physics of magnetic skyrmions, and in magnonics/spintronics in general.

I will discuss both general methods and their applications to electronic structure and magnetism of various groups of magnetic materials including elemental transition and rare-earth metals, half-metallic ferromagnets, transition metal oxides, molecular magnets, sp electron magnets based on adatoms on Si and SiC surfaces, and novel two-dimensional magnets.