AB INITIO THEORY OF EXCHANGE INTERACTIONS IN ITINERANT MAGNETS

I. Turek[a,b], J. Kudrnovský[c], V. Drchal[c], P. Bruno[d], and S. Blügel[e]

[a]Institute of Physics of Materials, Acad. Sci. Czech Rep., Brno, Czech Republic
[b]Dept. Electronic Structures, Charles University in Prague, Czech Republic
[c]Institute of Physics, Acad. Sci. Czech Rep., Prague, Czech Republic
[d]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany
[e]Institut für Festkörperforschung, Forchungszentrum Jülich, Germany

9.7 cm

The lecture reviews an efficient two-step procedure to determine magnetic properties of itinerant magnets from first principles. In the first step, the selfconsistent electronic structure of a system is calculated using the tight-binding linear muffin-tin orbital method combined with Green function techniques, which is appropriate for description of substitutional randomness of disordered bulk alloys and for two-dimensional translational periodicity of layered systems like surfaces and thin films. In the second step, the parameters of the effective classical Heisenberg Hamiltonian are determined using the magnetic force theorem and they are employed in subsequent evaluation of magnon spectra, the spin-wave stiffness constants and the Curie temperatures. Examples of application include: (i) ferromagnetic $3d$ metals Fe, Co, and Ni, (ii) disordered transition-metal alloys like bcc Fe-Co, (iii) ultrathin magnetic films of Fe and Co on a Cu(001) substrate, (iv) diluted magnetic semiconductors (Ga,Mn)As, and (v) f-electron systems like hcp Gd. The developed theory will be presented together with selected aspects of the numerical implementation and with a comparison to existing experimental data.

13.4 cm

Subject category :

6. Theory of Magnetism

Presentation mode :
oral (invited lecture)

Corresponding author :
I. Turek

Address for correspondence :
Institute of Physics of Materials,
Academy of Sciences of the Czech Republic,
Žižkova 22,
CZ-61662 Brno, Czech Republic

Email address :
turek@ipm.cz