TECHNISCHE UNIVERSITÄT WIEN
Vienna | Austria

INSTITUT FÜR FESTKÖRPERPHYSIK
Institute of Solid State Physics

Wiedner Hauptstr. 8-10/138, 1040 Wien
www.ifp.tuwien.ac.at

EINLADUNG zum IFP-SEMINAR

The standard model of the rare-earths in the Hubbard I approximation

Igor Di Marco

Department of Physics and Astronomy, Materials Theory,
Uppsala University, Uppsala, Sweden

Host:	Marco Battiato
Termin:	Montag, 28. November 2016, 15:30 Uhr
Ort:	Institut für Festkörperphysik, TU Wien
	Wiedner Hauptstraße 8-10, 1040 Wien
	Seminarraum DB gelb 07 (gelber Bereich, 7. OG)
Förderer:	FWF M1925-N28 FeMDy

In this talk I will present a critical analysis of the electronic properties of the rare-earth elements, by means of the Hubbard I approximation. Concerning the spectral properties, I will show that this approach is able to reproduce all measured (direct and inverse) photoemission features for basically all elements. Such a remarkable description of the electronic structure leads to cohesive properties (equilibrium volume and bulk modulus) in very good agreement with experimental data, especially if compared to previous theories. Moreover, basic magnetic properties such as spin and orbital moments are correctly described with the Hubbard I approximation, and compare well with data from the Curie-Weiss law and measurements of the high temperature susceptibility. In addition, we calculate the inter-atomic exchange parameters of an effective spin Hamiltonian for the heavy rare-earths. From those, ordering temperatures are obtained via Monte Carlo simulations and are shown to reproduce measurements with an error smaller than 10-30 K. The accuracy of these exchange parameters is also illustrated by comparing measured and calculated magnon dispersions for Gd. I will finally compare the Hubbard I approximation with other common theories of the electronic structure of the rare-earth elements, and highlight its (many) advantages and its (few) disadvantages. Alongside this comparison, I will illustrate our recent analysis of the stacking fault energies in Ce, including their relation to the hysteresis effects observed in the alpha-gamma transition cycle. In conclusion, I will also mention the relevance of the presented results to develop a generalized approach to treat the electronic structure of materials containing rare-earth elements, such as permanent magnets or molecular magnets.