SFB 608

Einladung zum Kolloquium

Ort: Universität zu Köln
II. Physikalisches Institut, Seminarraum 201

Zeit: Freitag!, 22. April 2005, 15 Uhr c.t.

Sprecher: Dr. Silke Biermann
Centre de Physique Théorique (CPHT)
École Polytechnique, 91128 Palaiseau Cedex, France

Thema: A dynamical mean field view on the electronic structure of correlated materials: "LDA+DMFT" and beyond.

The combination of dynamical mean field theory with electronic structure methods allows for the calculation of electronic properties of materials from first principles. We will describe some recent advances on transition metal compounds, in particular on the metal-insulator transition in VO_2 [1]. On the basis of our cluster dynamical mean field calculations we argue that Coulomb correlations are crucial for opening the gap in the insulating phase which, however, retains a strong Peierls character. Finally, we will also give a critical account of the "LDA+DMFT" technique and its shortcomings and discuss perspectives of how to go beyond [2].

[1] S. Biermann, A. Poteryaev, A. Lichtenstein, A. Georges, Phys. Rev. Lett. 94, 026404 (2005).

[2] S. Biermann, F. Aryasetiawan, A. Georges, Phys. Rev. Lett. 90, 086402 (2003), cond-mat/0401653 and cond-mat/0401626.

Gez. Prof. H. Tjeng