Electronic structure trends in transition metal oxides: the NMTO+DMFT approach

E. Pavarini

Institut für Festkörperforschung, Forschungzentrum Jülich, D-52425 Juelich, Germany

The combination of the first-principles N^{th}-Order Muffin-Tin Orbital (NMTO) method with a modern many-body technique, dynamical mean-field theory (DMFT), in short NMTO+DMFT method, is a powerful approach for elucidating *trends* in the properties of strongly correlated electron systems [1]. In this scheme *material-specific* Hubbard Hamiltonians – and the corresponding basis of Wannier functions – are constructed *ab-initio* by means of the NMTO downfolding technique; the small but realistic Hubbard models obtained with this procedure are then solved with DMFT. After an overview of the approach, as a striking example I will present the Mott metal-insulator transition and orbital-ordering phenomena in a family of $3d$ transition metal oxides [1, 2, 3].

[1] E. Pavarini, S. Biermann, A. Poteryaev, A.I. Lichtenstein, Georges A, and O.K. Andersen Phys. Rev. Lett. **92** 176403 (2004).
[2] E. Pavarini, A. Yamasaki, J. Nuss, O.K. Andersen, New J. Phys. **7**, 188 (2005).
[3] E. Pavarini, M. Raychaudhury, and O.K. Andersen, in preparation.