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Density Functional and Dynamical Mean-Field Theory (DFT+DMFT) method and its applications to correlation effects in electronic structure of real materials

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DATE / TIME	19.03.2012, 04:00 p.m. (CET)
LOCATION	Josef-Stefan-Hörsaal, vormals kleiner Hörsaal der Materialphysik, 3. Stock, Boltzmanngasse 5/Strudelhofgasse 4
ABSTRACT	DFT+DMFT method in Wannier functions realization is described. Application to a number of narrow-band materials is reported: SrVO3, V2O3, Li2VO4, NiO, MnO, FeSb2, LaOFeAs, KCuF3, Ce. Dynamical Mean-Field Theory (DMFT) is a powerful tool to study Coulomb correlations. To use it for real materials it should be combined with Density Functional Theory (DFT) methods. Wannier functions are used as localized orbitals basis to define Hamiltonian parameters. Coulomb interaction parameters are obtained in "constrained DFT" calculations. DFT+DMFT method was applied to a number of narrow-band materials where correlation effects result in anomalous physical properties: Strongly correlated metals SrVO3 Metal-insulator transition in V2O3 Heavy fermions in d-system Li2VO4 Charge transfer insulator NiO Metal insulator transition with pressure in MnO Correlated covalent insulators FeSi and FeSb2 Novel superconductor LaOFeAs Jahn-Teller distortions in KCuF3 f-electrons localization in Ce