Spring 12

Colloquium Cukrovarnická

**V pátek dne 16. března 2012 ve 14:00 hod.
ve Fyzikálním ústavu Cukrovarnická v seminární místnosti (budova A, 1. patro)**

DFT+DMFT method and its applications to correlation effects in electronic structure of real materials

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DFT+DMFT method in Wannier functions realization is described and its application to a number of narrow-band systems reported. The studied materials comprises $SrVO_3$, V_2O_3, Li_2VO_4, NiO, MnO, $FeSb_2$, LaOFeAs, $KCuF_3$, Ce. The dynamical mean-field theory (DMFT) is a powerful tool to study Coulomb correlations. In order to use it for real materials it should be combined with the density functional theory (DFT) methods. Wannier functions are used as localized orbital's 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 affects result in various anomalous physical systems: strongly correlated metals ($SrVO_3$), metal-insulator transition (V_2O_3, MnO), heavy fermions in d-system (Li_2VO_4), charge transfer insulator (NiO), correlated covalent insulators (FeSi, $FeSb_2$), novel superconductor (LaOFeAs), Jahn-Teller distortions ($KCuF_3$) or f-electrons localization (Ce).

J.J. Mareš, ved. sekce 3