LDA'+DMFT scheme: A way to treat the double counting problem

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We discuss the recently proposed LDA'+DMFT approach providing consistent parameter free treatment of the so called double counting problem arising within the LDA+DMFT hybrid computational method for realistic strongly correlated materials. In this approach the local exchange-correlation portion of electron-electron interaction is excluded from self consistent LDA calculations for strongly correlated electronic shells, e.g. d-states of transition metal compounds. Then the corresponding double counting term in LDA+DMFT Hamiltonian is consistently set in the local Hartree (fully localized limit - FLL) form of the Hubbard model interaction term. We present the results of extensive LDA'+DMFT calculations of densities of states, spectral densities and optical conductivity for most typical representatives of two wide classes of strongly correlated systems in paramagnetic phase: charge transfer insulators (MnO, CoO and NiO) and strongly correlated metals (SrVO3 and Sr2RuO4). It is shown that for NiO and CoO systems LDA'+DMFT qualitatively improves the conventional LDA+DMFT results with FLL type of double counting, where CoO and NiO were obtained to be metals. We also include in our calculations transition metal 4s-states located near the Fermi level missed in previous LDA+DMFT studies of these monooxides. General agreement with optical and X-ray experiments is obtained. For strongly correlated metals LDA'+DMFT results agree well with earlier LDA+DMFT calculations and existing experiments. However, in general LDA'+DMFT results give better quantitative agreement with experimental data for band gap sizes and oxygen states positions, as compared to the conventional LDA+DMFT. Also LDA'+DMFT method applied to the hole doped KFe2Se2 novel superconductor gives almost quantitative description of available ARPES data.