Band Calculation for f-electron systems on the basis of Dynamical Mean Field Theory

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The band calculation scheme for f electron compounds is developed on the basis of the dynamical mean field theory (DMFT) and the LMTO method[1]. The auxiliary impurity problem is solved by a method named as NCAf²v', which includes the correct exchange process of the $f^1 \rightarrow f^2$ virtual excitation as the vertex correction to the non-crossing approximation (NCA) for the $f^1 \rightarrow f^0$ fluctuation. This method leads to the correct magnitude of the Kondo temperature, T_K, and makes it possible to carry out quantitative DMFT calculation including the crystalline field (CF) and the spin-orbit (SO) splitting of the self-energy. The magnetic excitation spectra are also calculated to estimate T_K. It is applied to Ce metal and CeSb at T=300 K as the first step. In Ce metal, the hybridization intensity (HI) just below the Fermi energy is reduced in the DMFT band. The photo-emission spectra (PES) have a conspicuous SO side peak, similar to that of experiments, T_K is estimated to be about 70 K in γ-Ce, while to be about 1700 K in α-Ce. In CeSb, the double-peak-like structure of PES is reproduced. In addition, T_K which is not so low is obtained because HI is enhanced just at the Fermi energy in the DMFT band.

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