Temperature-dependent electron properties for 4f states in cerium mononitride

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Abstract

In order to elucidate the temperature-dependent valence state of Ce ion and the occupation number of Ce 4f electrons in cerium mononitride (CeN), we perform an ab initio calculation on CeN by using a many-body scheme combing density functional theory (DFT) with dynamical mean field theory (DMFT), taking into account the spin-orbit coupling (SOC) interaction and on-site Coulomb repulsion between Ce 4f electrons. Results demonstrate that Ce 4f j=5/2 and j=7/2 manifolds undergo insulating-metallic transition with the increasing of temperature. Ce 4f-conduction electrons hybridization, f-f correlation, SOC interaction and final state effects yield a complicated spectrum function in CeN. Ce 4f atomic configuration transition and hybridization might be responsible for the temperature-dependent occupancy number of Ce 4f electrons and the mixed-valence state in CeN. A fact that localization of Ce 4f electrons, i.e., 4f1 configuration or Ce3+ valence, increases with the increasing of temperature could account for the experimentally observed lattice constant versus temperature data. Finally, the so-called quasiparticle band structure is also discussed for comparison with experimental angle-resolved photoemission spectrum (ARPES).

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