ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES OF GdN - BULK AND SURFACE EFFECTS

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9.7 cm

The GdN crystallizes in a rocksalt structure and belongs to the family of rare-earth compounds which, due to the highly localized $4f$ orbitals, offer interesting magnetic properties for the field of spintronics. Although the electronic properties of GdN were studied previously the band structure of the compound is still under debate.

We present the results of the *ab initio* electronic structure calculations for bulk and surface of GdN carried out in ferromagnetic ground state with the Coulomb correlation interaction for the $4f$ manifold taken into account. The calculations were performed applying the Full Potential version of the Linearized Augmented Plane Wave method.

The GdN is strongly correlated electron system and to describe its thermodynamic properties we map it on the one-band Kondo-lattice model. Our aim was to elucidate the finite temperature electrical transport properties. We calculated the self-energy solving numerically equations for the single-electron Green functions. The set of paramters for the many-body Kondo-lattice model was based on the results of single-particle *ab-intio* calculations.

13.4 cm

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