Study of the Electronic Structure and Electric Field Gradient of Gadolinium Oxide in the Cubic Phase

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Abstract

In this work, the electronic properties of the cubic gadolinium oxide were investigated using the full-potential linearized augmented plane wave method in the density functional theory (DFT) framework. The calculations are performed within the generalized gradient approximation (GGA) while adding an empirical Hubbard U potential. The behavior of the electric field gradient (EFG) was analyzed and compared with the experimental data. Moreover, the total and partial densities of states of cubic Gd_2O_3 are presented and the contribution of different orbitals was determined in the total and partial density of states of curves. The calculations are in good agreement with the theoretical and experimental values.

Keywords: density functional theory, electric field gradient, Hubbard parameter, density of states, rare earth oxides, gadolinium oxide

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