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Crystal field and Ce^{3+} ion energy levels of $CeCl_3$ compound

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Abstract

In this paper, the crystal field parameters (CFPs) have been calculated in the framework of the density functional theory using a novel theoretical approach proposed by Pavel Novák et al. and extracting the WANNIER functions from the Bloch eigenstates for the $CeCl_3$ compound. Then, the calculated CFPs have been used in an effective atomic-like Hamiltonian, including the crystal field, 4f-4f correlation and spin-orbit coupling, and the splitted energy levels of Ce^{3+} ion by crystal field have been derived by diagonalization of the Hamiltonian. A hybridization parameter, , has been used to improve the results. The results are found to be in agreement with the experimental data.

Keywords: strongly correlated compounds, effective Hamiltonian, crystal field, density functional theory, WANNIER functions

For full article, refer to the Persian section