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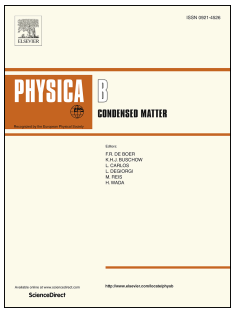

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Electronic response of rare-earth magnetic-refrigeration compounds GdX_2 (X= Fe and Co)

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Abstract

We present the Compton profiles (CPs) of rare-earth-transition metal compounds GdX_2 (X= Fe and Co) using 740 GBq ^{137}Cs Compton spectrometer. To compare the experimental momentum densities, we have also computed the CPs, electronic band structure, density of states (DOS) and Mulliken population (MP) using linear combination of atomic orbitals (LCAO) method. Local density and generalized gradient approximations within density functional theory (DFT) along with the hybridisation of Hartree-Fock and DFT (B3LYP and PBE0) have been considered under the framework of LCAO scheme. It is seen that the LCAO-B3LYP based momentum densities give a better agreement with the experimental data for both the compounds. The energy bands and DOS for both the spin-up and spin-down states show metallic like character of the reported intermetallic compounds. The localization of 3d electrons of Co and Fe has also been discussed in terms of equally normalized CPs and MP data. Discussion on magnetization using LCAO method is also included.