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Spin-Polarized Structural, Electronic and Magnetic Properties of Intermetallic Dy2Ni2Pb from Computational Study

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Abstract : We report a first-principles study of structural, electronic and magnetic properties of ternary plumbides (rare earth-transition metal-Plumb) Dy2Ni2Pb crystallizes with the orthorhombic structure of the Mn2AlB2 type (space group Cmmm), were studied by means of the full-relativistic version of the full-potential augmented plane wave plus local orbital method within the frame work of spin-polarized density functional theory (SP-DFT). The electronic exchange-correlation energy is described by generalized gradient approximation (GGA). We have calculated the lattice parameters, bulk modulii and the first pressure derivatives of the bulk modulii, total densities of states and magnetic properties. The calculated total magnetic moment is found to be equal to 9.52 μB.

Keywords : spin-polarized, magnetic properties, Dy2Ni2Pb, Density functional theory
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