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Calculated Structural and Electronic Properties of Mg and Bi

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Abstract : The present study shows the structural, electronic and magnetic properties of magnesium (Mg) and bismuth (Bi) in a supercell (1X1X5). For both materials were studied in five crystalline structures: rock salt (NaCl), cesium chloride (CsCl), zinc-blende (ZB), wurtzite (WZ), and nickel arsenide (NiAs), using the Density Functional Theory (DFT), the Generalized Gradient Approximation (GGA), and the Full Potential Linear Augmented Plane Wave (FP-LAPW) method. By means of fitting the Murnaghan's state equation we determine the lattice constant, the bulk modulus and it's derived with the pressure. Also we calculated the density of states (DOS) and the band structure.

Keywords : bismuth, magnesium, pseudo-potential, supercell
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