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First-Principles Investigation of the Structural and Electronic Properties of Mg1-xBixO

Authors : G. P. Abdel Rahim, M. María Guadalupe Moreno Armenta, Jairo Arbey Rodriguez

Abstract : We investigated the structure and electronic properties of the compound Mg1-xBixO with varying concentrations of 0, ¼, ½, and ¾ x bismuth in the the NaCl (rock-salt) and WZ (wurtzite) phases. The calculations were performed using the first-principles pseudo-potential method within the framework of spin density functional theory (DFT). Our calculations predict that for Bi concentrations greater than ~70%, the WZ structure is more favorable than the NaCl one and that for x = 0 (pure MgO), x = 0.25 and x = 0.50 of Bi concentration the NaCl structure is more favorable than the WZ one. For x = 0.75 of Bi, a transition from wurtzite towards NaCl is possible, when the pressure is about 22 GPa. Also It has been observed the crystal lattice constant closely follows Vegard's law, that the bulk modulus and the cohesion energy decrease with the concentration x of Bi.

Keywords : DFT, Mg1-xBixO, pseudo-potential, rock-salt, wurtzite
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