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Characterization of Nickel Based Metallic Superconducting Materials

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Abstract : Density functional theory is used to investigate the.the structural, electronic, and magnetic properties of the cubic anti-perovskites InNNi3 and ZnNNi3. The structure of antiperovskite also called (perovskite-inverse) identical to the perovskite structure of the general formula ABX3, where A is a main group (III–V) element or a metallic element, B is carbon or nitrogen, and X is a transition metal, displays a wide range of interesting physical properties, such as giant magnetoresistance. Elastic and electronic properties were determined using generalized gradient approximation (GGA), and local spin density approximation (LSDA) approaches,), as implemented in the Wien2k computer package. The results show that the two compounds are strong ductile and satisfy the Born-Huang criteria, so they are mechanically stable at normal conditions. Electronic properties show that the two compounds studied are metallic and non-magnetic. The studies of these compounds have confirmed the effectiveness of the two approximations and the ground-state properties are in good agreement with experimental data and theoretical results available.

Keywords : anti-perovskites, elastic anisotropy, electronic band structure, first-principles calculations
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