$InNCo_3$ and $InNNi_3$ with cubic anti-perovskite structure, we carried out the first-principles calculations on these compounds using the pseudopotentials method with plane-wave basis set within the local density approximation and the generalized gradient approximation. Since the elastic properties of a solid are highly associated with various fundamental solid-state properties such as phonon spectra, specific heat, Debye temperature, and so on, we have calculated the independent elastic constant and the elastic moduli of $InNCo_3$ and $InNNi_3$.

II. COMPUTATIONAL DETAILS

All calculations on antiperovskite-type $InNCo_3$ and $InNNi_3$ were performed using the Quantum ESPRESSO code[20], which is based on the density functional theory (DFT)[21]. The electronic exchange-correlation potential was calculated within the local density approximation (LDA)[22,23] and the generalized gradient approximation using the scheme of Perdew-Burke-Ernzerhof (PBE)[24]. The spin polarization was also considered in the calculation in order to assess the magnetic properties of these compounds. Electron-ion interaction was represented by the norm-conserving optimized[25] designed nonlocal pseudopotentials. The $4d$ electrons are explicitly included in the valence of In. The electronic wavefunctions were expanded by the plane waves up to a kinetic energy cutoff of 55 Ry. The **k**-point sampling in Brillouin zone (BZ) of simple cubic lattice was treated with the Monkhorst-Pack scheme[26] and a 20×20×20 **k**-point mesh (i.e., 286 irreducible points in the first BZ) was used. The chosen plane-wave cutoff and number of **k** points were carefully checked to ensure that the total energy was converged to be better than 1 mRy/cell. The total energies are obtained as a function of volume and they are fitted with the Birch-Murnaghan 3rd-order equation of states (EoS)[27] to give the equilibrium lattice constant and other ground state properties. During the calculation of density of states (DOS), a dense **k**-point mesh of 30×30×30 is used, the total DOS is computed by the tetrahedron method[28], and the atomic-projected DOS is calculated by the Löwdin populations[29].

For a cubic crystal, its independent elastic constants are c_{11}, c_{12}, and c_{44}. To determine the elastic constants of $InNCo_3$ and $InNNi_3$ by means of the curvature of the internal energy versus the strain curves[30,31], three strain modes[32] are adopted and their nonzero strains are as follows: (1) $\epsilon_{11} = \epsilon_{22} = \delta$, $\epsilon_{33} = (1+\delta)^{-2} - 1$; (2) $\epsilon_{11} = \epsilon_{22} = \epsilon_{33} = \delta$; and (3) $\epsilon_{12} = \epsilon_{21} = \delta/2$, $\epsilon_{33} = \delta^2/(4-\delta^2)$. The deformation magnitudes δ from -0.012 to 0.012