$InNCo_3$ and $InNNi_3$ play dominant roles in the total dnesity of states of these compounds.

In order to understand the bonding nature among the ions in $InNCo_3$ and $InNNi_3$, we analyzed the charge density contours of $InNCo_3$ and $InNNi_3$ in the(110) plane, as shown in Fig. 4. From Fig. 4, it is found that a certain amount of charges are accumulated in the intermediate region between N and Co atoms in $InNCo_3$, and slightly more charges are accumulated intermediate region between N and Ni atoms in $InNNi_3$. This gives an evidence for the strong hybridization between N and transition metal (Co/Ni) atoms, indicating that the N-Co and N-Ni bondings exhibit strong covalent characteristics and the latter is slightly stronger than the former. The similar bonding characteristics for Ni-N atoms or Ni-C atoms were also found in other Ni-based ternary nitrides or carbides $AXNi_3$[10,14,37,38]. Therefore, our results suggest that the magnetic properties of $InNNi_3$ reported in experiment[15] are very likely due to the non-stoichiometry effect, which was also found in the cases of $AlCNi_3$ and $GaCNi_3$[12,16–19].

IV. CONCLUSIONS

In summary, we performed the first-principles calculations to study the elastic and electronic properties of cubic antiperovskites $InNCo_3$ and $InNNi_3$. Based on the Voigt, Reuss and Hill bounds, the shear, Young's moduli and Poisson's ratio have also been estimated for the $InNCo_3$ and $InNNi_3$ polycrystals. The theoretically predicted equilibrium lattice parameters are in good agreement with the available experimental data. Our calculations show that the $3d$ states of transition metal atoms in $InNCo_3$ and $InNNi_3$ play dominant roles near the Fermi levels. $InNCo_3$ energetically prefers to the ferromagnetic state. The magnetic ground state of $InNNi_3$, which is same to other Ni-based ternary nitrides or carbides with a cubic anti-perovskite structure, is a stable paramagnetic (non-magnetic) state. This could be understood from that the hybridization between Ni-$3d$ and N-$2p$ states in $InNNi_3$ is slightly stronger than the one between Co-$3d$ and N-$2p$ states in $InNCo_3$ because of the more $3d$ electrons in Ni.