I. INTRODUCTION

The ternary nitrides or carbides with the general formula AXM_3 (A: divalent or trivalent element; X: carbon or nitrogen; and M: transition metal) are already known for several decades [1–3]. These compounds crystalize in a cubic anti-perovskite structure (A: cube-corner position; X: body-center position; M: face-center position) and exhibit a wide range of interesting physical properties[1], such as giant magneto-resistance[4] and nearly zero temperature coefficient resistivity[5]. They have renewedly attracted considerable attention due to the discovery of superconductivity at $\sim$8 K in intermetallic compound $MgCNi_3$[6].

Considering the Ni-rich composition, it is expected that the ferromagnetism could exist in $MgCNi_3$. However, the absence of ferromagnetism was observed in experiment[6] for $MgCNi_3$. From the electronic structures obtained by the first-principles calculations[7–10], the non-ferromagnetic ground state of $MgCNi_3$ is ascribed to a reduced Stoner factor that results from a strong hybridization between the Ni-3d and C-2p electrons. For other Ni-based ternary carbides $ACNi_3$ (e.g., A = Al, Ca, In, Zn, and Cd), the first-principles calculations[10–14] also show that the ground states of these compounds are non-magnetic and the C-Ni bonding exhibits nearly same characteristics as the one in $MgCNi_3$. Therefore, this indicates that the change of composition A could not induce the ferromagnetism in $ACNi_3$. On the other side, it raises a question whether the change of composition X or M can lead to the appearance of ferromagnetism in AXM_3 or not.

Very recently, the antiperovskite-type compounds InN_yCo_3 and InN_yNi_3 ($y \sim 1.0$ and 0.8, respectively) have been synthesized by solid-gas reactions of metal powders with NH_3 and they have been reported to have spin-glass-like properties based on the measurements of temperature dependence magnetization.[15] The recent first-principles calculations[12] showed that the non-stoichiometry could affect the magnetic properties of $ACNi_3$ (e.g., $AlCNi_3$ and $GaCNi_3$) and suggested that the tendencies toward magnetism found in experiments[16–19] for these compounds should be explained by the deviation of the Ni/C atomic ratio from the ideal stoichiometry. To shed more light on the understanding on the magnetic properties of $InNCo_3$ and $InNNi_3$ reported in experiment[15], it is of great importance to theoretically study the electronic structures of these two compounds as well as the nature of the N-Co and N-Ni bondings.

In order to completely understand the electronic structures and magnetic ground states of