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First-principles study of cobalt pnictide $SrCo_2N_2$ ANDREW O'HARA, ALEXANDER DEMKOV, The University of Texas at Austin — With the recent discovery of high temperature superconductivity in $BaFe_2As_2$, there has been renewed interest in other members of the AT_2X_2 family (A = alkaline earth element or lanthanide, T = transition metal, X = an element of groups IIIB-VIB) and in particle isovalent members of the 122 family. In this work, we describe a hypothetical cobalt pnictide, SrCo2N2, using density functional theory (DFT) in the local density approximation (LDA) with a Hubbard U correction. In this work, we determine both the lattice and chemical stability of $SrCo_2N_2$ as well as explore how the substitutions affect the electronic and magnetic properties in comparison to $BaFe_2As_2$ and 122 rare-earth cobalt phosphides.

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