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First-principles study of cobalt pnictides: Example compound $SrCo_2N_2$ ANDREW O'HARA, ALEXANDER DEMKOV, The University of Texas at Austin — Although it has been known for several decades that many materials with chemical form AT_2X_2 (A = alkaline earth element or lanthanide, T = transition metal, X = an element of groups IIIB-VIB) crystallize with the same structure, it was only recently that interest was renewed in these materials with the discovery that $BaFe_2As_2$ can be made to superconductor at temperatures as high as 38 K. Although the precise mechanism of superconductivity has yet to be determined, there is a growing interest in the study of materials that have similar electronic properties to $BaFe_2As_2$. In our work, we employ density functional theory in the local density approximation in order to study the isochemically substituted variant, $SrCo_2N_2$. In this work, we determine both the stability of $SrCo_2N_2$ as well as how the substitution changes the electronic properties in comparison to $BaFe_2As_2$.

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