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Density-Functional Calculations of the Electronic Structures and Magnetism of the Pnictide Superconductors $BaFeAs_2$ and $BaFeSb_2$

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We investigate the structural, electronic, and magnetic properties of the hypothetical compound $BaFePn_2$ (Pn=As and Sb), which is isostructural to the parent compound of the high-temperature superconductor $LaFeAsO_{1-x}F_x$. Using density-functional theory, we show that the Fermi surface, electronic structure, and spin-density wave instability of $BaFePn_2$ are very similar to the Fe-based superconductors. Additionally, there are very dispersive metallic bands of a spacer Pn layer, which are almost decoupled from FePn layer. Our results show that experimental study of $BaFePn_2$ can test the role of charge and polarization fluctuation as well as the importance of two dimensionality in the mechanism of superconductivity. We will also discuss the role of strongly correlated electrons in these compounds.