Abstract Submitted
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First Principles Study of Electronic and Vibrational Properties of $BaHfN_2$[1] AMANDEEP KAUR, ERIK YLVISAKER, Department of Physics, University of California, Davis, USA, YAN LI, GIULIA GALLI, Department of Chemistry, University of California, Davis, USA, WARREN PICKETT, Department of Physics, University of California, Davis, USA — The transition metal nitride $BaHfN_2$, which consists of weakly bonded neutral slabs of closed shell ions, has structural and chemical similarities to other layered nitrides which have impressive superconducting T_c's when electron doped: A_xHfNCl, A_xZrNCl, A_xTiNCl, with T_c= 26, 15.5 and 16 K, respectively for appropriate donor (A) concentrations x. These similarities suggest that $BaHfN_2$ may exhibit relatively high T_c upon doping, with effects of structure and the role of specific transition metal ions yet to be understood. We carried out electronic structure calculations for stoichiometric $BaHfN_2$ and found a direct band gap of about 0.8 eV within Density Functional Theory, using the local density approximation. Doped electrons are expected to occupy the lowest conduction band, which has primarily Hf $5d_{xy}$ character (similar to α-TiNCl which has the lowest conduction band primarily composed of Ti $3d_{xy}$). We also find that the two N sites, N1 in the Hf layer and N2 in the Ba layer, have very different Born effective charges (BEC). The deviations from the formal (-3) charge are opposite for the two sites. Comparison to the BEC's of the other compounds, and to the LO-TO splitting, will be discussed.

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