Abstract Submitted
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Electronic and defect structure of CuSCN[1] JOHN JAFFE, TIFFANY KASPAR, TIMOTHY DROUBAY, Pacific NW National Lab — We calculate the band structure, bonding characteristics and basic native defect configurations of hexagonal copper thiocyanate, β-CuSCN, for the first time. β-CuSCN is predicted to be an indirect-gap semiconductor with an unusual orbital character: While the highest valence bands have the expected character of Cu-3d levels hybridized with sulfur 3p states, the conduction band minimum (at the K point of the hexagonal Brillouin zone) has mostly cyanide antibonding character. This quasi-molecular character results in some unusual properties, including electron effective masses that are comparable to or even larger than the hole effective masses. However, optical absorption measurements on polycrystalline films do not support the indirect nature of the lowest transitions, though they also do not clearly contradict it. The dominant p-type character of this material is explained in terms of copper vacancies, possibly augmented by CN unit vacancies, which are expected to be acceptors. By contrast, a vacancy of a complete SCN unit would be a donor, but is not expected to occur at significant concentrations in this material.

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