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Electronic properties of ultra-wide-band-gap nitride alloys from first principles[1] JIMMY-XUAN SHEN, DARSHANA WICKRAMARATNE, CHRIS VAN DE WALLE, Univ of California - Santa Barbara — Boron-containing nitride alloys such as BAlN and BGaN are being explored as novel members of the nitride family for electronic and optoelectronic applications. The design of materials and devices for such applications requires a fundamental understanding of the composition-dependent electronic structure. At low B content, the materials stabilize in the wurtzite structure; BN itself is not stable in the wurtzite structure, and therefore no experimental information is available to allow predictions for the B-containing alloys. In this work, we employ density functional theory with a hybrid functional to investigate the electronic structure of B-containing alloys as a function of boron content. Wurtzite BN is an indirect band-gap semiconductor, while AlN and GaN have a direct band gap; we therefore expect a crossover from direct to indirect band gap as a function of increasing B content. We also expect large band-gap bowing due to the large lattice mismatch between the parent compounds. We are able to accurately identify the direct-to-indirect crossover by using a projection scheme. We find that the bowing parameter for the direct band gap is much larger than for the indirect gap. We also investigate the sensitivity of these properties to the B distribution.

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