

Abstract Submitted  
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**Structural and electronic properties of BAlN alloy**<sup>1</sup> JIMMY-XUAN SHEN, Dept. of Physics Univ of California - Santa Barbara, DARSHANA WICKRAMARATNE, CHRIS G VAN DE WALLE, Materials Dept., UC Santa Barbara — Designs of far-UV emitters using BAlN as the barrier layer and AlN as the active layer are being considered. Realization of BAlN alloys is complicated by the fact that BN is most stable in a hexagonal structure, which is different from the ground-state wurtzite structure of AlN. Enabling such designs requires a fundamental understanding of the composition dependent electronic structure of BAlN. Using first-principles simulations based on a hybrid functional, we investigate the band gaps, band-gap bowing, and miscibility of BAlN using explicit alloy calculations. The results from these calculations are used to determine the band offsets between AlN and BAlN that are essential to assess the performance of UV-emitting devices.

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