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Prospects and limitations for p-type doping in boron nitride polymorphs[1] LEIGH WESTON, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Using first-principles calculations, we examine the potential for p-type doping of BN polymorphs via substitutional impurities. Based on density functional theory with a hybrid functional, our calculations reveal that group-IV elements (C, Si) substituting at the N site result in acceptor levels that are more than 1 eV above the valence-band maximum in all of the BN polymorphs, and hence far too deep to allow for p-type doping. On the other hand, group-II elements (Be, Mg) substituting at the B site lead to shallower acceptor levels. However, for the ground-state hexagonal phase (h-BN), we show that p-type doping at the B site is inhibited by the formation of hole polarons. Our calculations reveal that hole localization is intrinsic to sp^2 bonded h-BN, and this places fundamental limits on hole conduction in this material. In contrast, the sp^3 bonded wurtzite (w-BN) and cubic (c-BN) polymorphs are capable of forming shallow acceptor levels. For Be dopants, the acceptor ionization energies are 0.31 eV and 0.24 eV for w-BN and c-BN, respectively; these values are only slightly larger than the ionization energy of the Mg acceptor in GaN.

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