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**Defect and Impurity Properties of Hexagonal Boron-nitride** BING HUANG, SU-HUAI WEI, National Renewable Energy Lab — By using both GGA and hybrid functional calculations, we have systematically calculated the properties of defects and impurity in hexagonal boron-nitride ($h$-BN). Our calculations show that the defect configurations and the local bond lengths around defects are sensitive to their charge states. The possible highest negative charge states of defects are largely determined by the nearly- free-electron state at the conduction band minimum. The in-gap defect levels got from hybrid functional calculations are much deeper than those got from GGA calculations. The formation energies of neutral defects calculated by hybrid functional and GGA are close to each other, but the defect transition energy level between charge states and neutral state respect to valence band maximum are quite different in GGA and hybrid functional calculations. Finally, we show that the charged defect configurations as well as the transition energy levels exhibit interesting layer effects.

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