Electronic Structures of 4H-SiC with Group I and VII Elements: First-Principles Study of Possible p-Type Doping

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On the basis of first-principles calculations, we investigated the total energies and electronic structures of 4H-SiC containing group I and VII elements (H. Li, Na, K, and Rb from group I, and F, Cl, Br, and I from group VII) as impurities. We determined the favorable site, ionization energy and defect concentration for each impurity in 4H-SiC. It was found that the formation energies of H and Li interstitial sites are always lower than those at substitutional sites. In particular for F and Na, the higher stability at either interstitial or substitutional site depends on C-rich condition. Our calculation revealed that the interstitial F introduces a rather shallow acceptor level as well as conventional p-type dopants such as B and Al at substitutional Si sites. This suggests that the interstitial F can be used to fabricate low-resistivity p-type SiC.