Theoretical Study of Acceptor–Donor Complexes in 4H-SiC

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The total energies and electronic structures of acceptor-donor complexes in 4H-SiC were investigated using *ab initio* calculation methods. Our calculations covered the A_2D complex consisting of substitutional two-acceptor atoms from group-III elements and a nitrogen (N) donor atom. Results indicate some A_2D complexes can exist stably, and solid solubilities of Al_2N and Ga_2N may be greatly enhanced. We also found that Ga_2N introduces a shallower acceptor level compared to conventional acceptor atoms such as B and Al. Our results suggest that Ga^+/N^+ co-implantation is one of the promising candidates for a doping method to realize low-resistivity p-type 4H-SiC.