Electronic Structures of Semiconductor Clusters with Point Defects (19)

Yoshitsune Higashiguchi, Kazuyuki Igei, Hiroaki Ochiai, Yoshinori Hayafuji

Ab initio calculations of the atomic and the electronic structures of crystalline silicon (c-Si) with $X@B_6$ and $X@B_{12}$ (X=H-Br) clusters have been performed to investigate carrier generation by dopant atoms inside in cage of boron clusters. It is found that B_{12} and B_6 can exist stably in c-Si and should act as a double acceptor. It is also found that H, Be, B, Cr and Mn atoms can be settled in the cubo-octahedral B_{12} cluster and especially H atom can introduce a very shallow acceptor level. The $H@B_{12}$ cluster is one of the most promising candidates as a cluster dopant for the formation of a high-performance extremely shallow junction in the future ULSI.