# A mechanism for hole generation by octahedral $B_6$ clusters in silicon

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The electronic structure and x-ray photoelectron spectra of silicon with octahedral $B_6$ clusters are investigated using first-principles calculations. It is found that the $B_6$ clusters act as double acceptors in silicon and that the simulated chemical shift of the B 1*s* orbital signals of the $B_6$ clusters in x-ray photoelectron spectra coincides with the chemical shift of B 1*s* experimentally observed in as-implanted silicon at an extremely high dose of boron. These results reveal that the $B_6$ clusters are the origin of hole carries. We propose a mechanism of hole generation and a model of $B_6$ cluster formation at implantation-induced divacancy sites.