Atom-vacancy Effect on Band structure and optical conductivity of $Ga_{0.9375}$ $Al_{0.0625}As$

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Band structure of $Ga_{0.9375}Al_{0.0625}As$ with Ga and As monovacancies are analyzed with density functional theory (DFT) caculation. We have introduced eight types of monovacancies, which change electrical properties of the material. Other properties include atomic charges, density of states (DOS), orbital structures, and optical conductivity. We found that all band gaps become narrower upon introducing vacancy. Also, Fermi level enters into the valence band so that the vacant materials may show the characteristics of the p-type semiconductor. Interestingly, Ga-vacancy systems make direct band gaps, whereas As-vacancy systems make indirect gaps. The latter phenomenon is induced by the separation of initial band structures near Fermi level, of which the identity is the overlapping of hybridised 4s and 4p orbitals of Ga atoms around As vacancy, and this newly formed state could lead to electron hopping from the valence band but this results in the loss of semiconducting nature.