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A bound exciton model of acceptors in semiconductors YONG ZHANG, JIANWEI WANG, University of North Carolina at Charlotte — We point out that the electronic structure of an acceptor bears a close similarity to that of an isoelectronic impurity bound exciton with a larger electronegativity (known as "acceptor-like bound exciton") [Hopfield et al., PRL 17, 312(1966)], and to some extent to that of a free exciton in a semiconductor. Instead of using only one quantity ***acceptor binding energy*** E_A (based on Coulomb interaction) when dealing with the electronic transitions involving an acceptor, another quantity ***impurity binding energy*** E_I, depending on the atomic orbital difference, is usually more important in the transition processes. E_I resembles the role of the electron bound state or conduction band edge, whereas E_A resembles the hole or exciton binding energy, respectively, in the isoelectronic impurity or free exciton case. Furthermore, instead of viewing the acceptor impurity as a "shallow impurity" and isoelectronic impurity as a "deep impurity", it would be more appropriate to view for both impurity types that the bare electron bound state involves a localized potential, and the ionized impurity has a long-range Coulomb potential. A first-principles calculation of the total energy difference yields approximately $E_I - E_A$, but the energy needed to generate free holes is in fact E_I.

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