

Diagonal parameter shifts in strained semiconductors in the empirical tight-binding theory

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Many empirical tight-binding models require adjustment to the diagonal parameters in order to correctly reproduce the behavior of the band edges under uniaxial strain. These adjustments typically take the form of one or two additional parameters which shift the p- and/or d-onsite parameters. Such adjustments, while satisfactory in the case of uniaxial strain, are of little use in nano-structure models, where the atoms can be irregularly positioned. To address this case we present our method for determining the diagonal parameter shifts in the case of arbitrary atomic displacements. Our results agree well with other available experimental or theoretical data for the cases of uniaxial and hydrostatic strain, yet are not at all restricted to these situations.