

Ab initio determination of deformation potentials of tetrahedral semiconductors

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Coherent lattice strain may be used to deliberately alter the band structure of a semiconductor by altering the fundamental gap or splitting electronic states normally degenerate due to crystal symmetry. The parameters which describe the relationship between lattice strain and the electronic band structure are known as deformation potentials (DP's). The accurate investigation of these quantities is important for understanding the band structure of semiconductor devices. Calculations performed using phenomenological (empirical) methods as well as the experiment show a significant spread in the reported values for tetrahedral semiconductors. Therefore, it appears necessary to perform a consistent first-principles investigation of the most used semiconductors. In this work, we report on *ab initio* calculations of the DP's induced both from lattice-strain and zone-center acoustic phonon deformations for several tetrahedral semiconductors. The electronic band structure has been calculated using the plane-wave pseudopotential method within density-functional theory in the local-density approximation. Then, the DP's are calculated as suitably symmetrized linear coefficients of the variation of band-structure eigenvalues with respect to macroscopic strain or acoustic-phonon relative displacements. Finally, the results are analyzed in order to discuss possible trends in the behavior of the DP's.