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First-principles calculations of structural, electronic and optical properties of Zinc-blende $Si_x Ge_{1-x} C$ alloys

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Abstract: We present first-principles calculations of the structural, electronic and optical properties of zinc-blende $Si_x Ge_{1-x} C$ alloys by application of the full potential linearized augmented plane wave (FP-LAPW) method. In this approach, the generalized gradient approximation was used for the exchange-correlation energy which is based on the optimization of total energy and corresponding potential. The effect of composition on lattice constants, bulk modulus, band gap, real part of the dielectric function \varepsilon \left(0 \right) and refractive index n(0) was investigated. These parameters were found to depend nonlinearly on alloy composition x, except the bulk modulus and the lattice parameter, which follows Vegard's law. Using the approach of Zunger et al, the microscopic origin of the gap bowing is also elucidated. It is concluded that the energy band gap bowing is primarily due to chemical charge-transfer effect. Contribution of volume deformation and structural relaxation to the gap bowing parameter is found to be very small.

Key Words: Alloys, Lattice parameter, Bulk modulus, Electronic structure, Band-gap, Gap bowing, Optical properties.

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