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Electronic structure of random Alp 5Gao.5As alloys: Test of the "special-quasirandom-structures" description

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The spectral properties of an sp's tight-binding Hamiltonian for a random, unrelaxed A10.5Ga0.5As alloy are calculated using three diferent techniques: the coherent-potential

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parameter that allows us to vary the differences between
Al and Ga diagonal parameters from zero (VCA) to that
of the crystalline parametrizations (X=1) and beyond.
Since we are primarily interested in a comparison of
different theoretical predictions, we will not concern our-
selves with the question of how accurately the present model describes Aln 5Gan sAs. It is sufficient for our pur-poses that Eq. (1) provides reasonable valence and lower
conduction bands and a range of scattering strengths. "
(For l 1, the Ga s, p, and s levels differ from those of Al by —1.02, +0.55, and +0.48 eV, respectively.) For reference, we list in the first two columns in Table I the I ~, X~, and Xi conduction-band eigenvalues obtained by replacing the cation diagonal parameters in HvcA by their values in GaAs and A1As, respectively. ' The absolute VCA energies

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TABLE I. Top: Location of spectral features (in eV) associated with the zinc-blende I ~, X~, and X3 states. The first two columns are obtained by replacing the cation diagonal parameters in the VCA Hamiltonian by their GaAs and AlAs values, respectively. Entries for