as a function of volume V. Here, $y_{a\,strd}$ is the screened, strain-dependent nonlocal pseudopotential of atom type a (e.g., In, P, or passivant) fitted [11] to the measured bulk band structure and effective masses, and to the calculated [via local density approximation (LDA)] deformation potentials and charge densities. Using our pseudopotentials the calculated *absolute* InP deformation potentials are 21.39, 27.73, 10.88, and 23.38 eV for G_{15y}, G_{1c}, X_{1c}, and L_{1c}, respectively, while the *ab initio* LAPW (linearized augmented plane wave) values [12] are 21.00, 26.26, 10.65, 23.30 eV, respectively. The measured [13,14] *relative* $G_{1c}-G_{15y}$ and $X_{1c}-G_{15y}$ deformation potentials are 26.40 and 12.20

Thus, the X_{1c}-G_{1c} energy difference is reduced in this dot by 0.27 eV relative to the bulk value.

Interestingly, (i) the confinement energies $De_g(V)$ are nearly pressure independent. They are 0.28 (0.60) eV at the transition volume $V > 0.93V_{eq}$, and 0.31 (0.58) eV at V_{eq} for the X_{1c} (G_{1c}) state of the $D > 34.8$ Å dot. This suggests that the reduced size affects the dot's wave function *macroscopically* (i.e., by altering the envelope part), while the pressure affects the wave function *microscopically* (by changing the periodic Bloch part). The fact that the confinement energies are close for the zero-pressure dot and for the compressed dot, provides one way to obtain the quantum size effect on those states at Brillouin-zone edge, which proved to be difficult under ambient pressure [17]. (ii) The X_{1c} confinement energy obtained in our direct diagonalization approach [Eq. (1)] is surprisingly *larger* than what was expected from effective-mass approximation (EMA): using the calculated effective masses [11] $m_e^p(G_{1c}) > 0.095$, $m_e^p(X_{1c}) > 2.04$, the EMA gives 0.06 (1.31) eV for the confinement energy of X_{1c}-like (G_{1c}-like) conduction state. Thus, the EMA predicts that the $G \rightarrow X$ transition will already occur at zero pressure for this $D > 34.8$ Å dot. Actually, we find that an accurate description of the *whole* lowest bulk conduction band (not just near G and *X* as in the EMA) is needed to predict the correct G-*X* energy separation (thus the critical pressure) in dots. (iii) Our calculations further show that the reduction of G-*X* energy separation relative to the bulk value is not a simple monotonic function of dot size (the reduction is 0.15, 0.27, and 0.00 eV for $D > 20.2$, 34.8, and ∞ Å dots, respectively). (iv) One interesting issue regarding InP dots is the envelope-function symmetry of the top valence state. We find that the envelope is *s*-like both at zero pressure and near the transition pressure. This is consistent with point (i) that the pressure does not change the property due to envelope difference.

To understand the level crossings and anticrossings evident in Fig. 3 we consider the symmetries of the states of the bulk and the dots (Table II). In the diamondlike bulk band structure, the lowest *X* conduction state is twofold degenerate (neglecting spin), while in zinc-blende band structure, it is broken into two singly degenerate states

TABLE II. Symmetries of the G-like, *X*-like, and *L*-like conduction states in bulk InP and in InP dots with different atoms at the dot center. Overbar denotes the state in the dot while its bulk parentage is given in parentheses.

Bulk states	Anion-centered	Cation-centered
G_{1c}	$\overline{G}_{1c}(G_{1c})$	$\overline{G}_1$

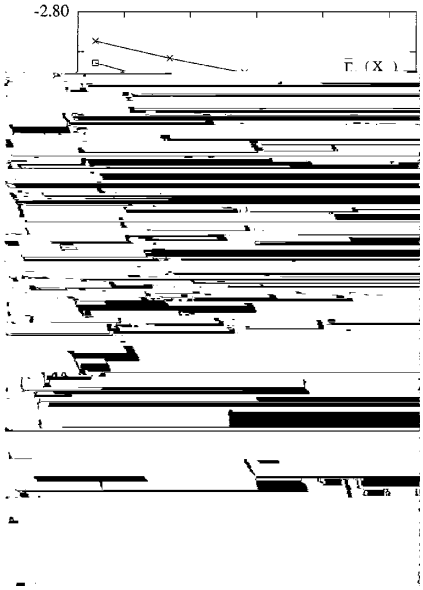

FIG. 5. Variation of the near-edge conduction states $\overline{\Gamma}_{1c}(\Gamma_{1c})$, $\overline{\Gamma}_{1c}(L_{1c})$, $\overline{\Gamma}_{15c}(L_{1c})$, and $\overline{\Gamma}_{15c}(X_{1c})$ of In-centered InP dots with lattice compression near the critical point: (a) $D > 20.2$ Å dot; (b) $D > 34.8$ Å dot.

bulk, 3.3 meV for $D > 34.8$ Å dot, and 34.2 meV for $D > 20.2$ Å dot. The size scaling of Γ-X coupling is $V_{\Gamma X} \sim 1/D^{l}$ with $l > 4.30$. This shows that reduction in quantum size enhances dramatically interstate coupling. Our Γ-X coupling values are much larger than the values