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Pressure effects on neutral and charged excitons in self-assembled (In,Ga)As/GaAs quantum dots

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By combining an atomistic pseudopotential method with the configuration-interaction approach, we predict the pressure dependence of the binding energies of neutral and charged excitons: X^0 (neutral monoexciton), X^- and X^+ (charged trions), and XX^0 (biexciton) in lens-shaped, self-assembled $In_{0.6}Ga_{0.4}As/GaAs$ quantum dots. We predict that (i) with applied pressure the binding energy of X^0 and X^+ increases and that of X^- decreases, whereas the binding energy of XX^0 is nearly pressure independent. (ii) Correlations have a small effect in the binding energy of X^0, whereas they largely determine the binding energy of X^-, X^+, and XX^0. (iii) Correlations depend weakly on pressure; thus, the pressure dependence of the binding energies can be understood within the Hartree-Fock approximation and it is controlled by the pressure dependence of the direct Coulomb integrals J. Our results in (i) can thus be explained by noting that holes are more localized than electrons, so the Coulomb energies obey $J^{(hh)}>J^{(eh)}>J^{(ee)}$.

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The energetics of excitons reflects a balance between single-particle energy levels $\mathcal{E}^{(e)}$ and $\mathcal{E}^{(h)}$ of electrons (e) and holes (h) in the system, and the many-particle carrier-carrier interactions resulting from electron-hole Coulomb and exchange interactions.[1–3] The variation of excitonic energies under pressure naturally reflects the corresponding variations in single- versus many-particle energies. Of particular interest are the pressure variations of excitons confined to nanosize dimensions such as in quantum dots.[4–14] Unlike the case of excitons in higher-dimensional systems, where binding and its pressure dependence reflects mostly many-particle (correlation) effects, in zero-dimensional (0D) systems where the geometric dimensions are smaller than the excitonic radius, binding of neutral and charged excitons results from an interesting *interplay* between single-particle and many-particle effects. Here, we use a realistic description of both single-particle and many-body effects in self-assembled $In_{0.6}Ga_{0.4}As/GaAs$ quantum dots, showing how pressure affects the different components of exciton binding. We distinguish the neutral monoexciton X^0 (one e, one h), from the neutral biexciton XX^0 (two e, two h), positive trion X^+ (one e, two h), and negative trion X^- (two e, one h). While the effect of pressure on X^0 has been measured,[8–14] to the best of our knowledge, the optical spectroscopy of X^-, X^+, and XX^0 under pressure has not yet been reported. Each of the q-charged excitons has a spectrum of levels $\{\nu\}$, of which the lowest is termed the "ground state of χ^q" ($\chi=X,XX$). This spectrum is usually expressed by expanding the many-body excitonic states $|\Psi^{(\nu)}(\chi^q)\rangle$ via a set of Slater determinants $|\Phi(\chi^q)\rangle$. The latter are constructed from single-particle electron and hole states and accommodate as many carriers as are present in χ^q. The single-particle states are solutions to the effective Schrödinger equation

$$\left\{-\tfrac{1}{2}\nabla^2+V_{\rm ext}(\mathbf{R})+V_{\rm scr}(\mathbf{R})\right\}\psi_i=\mathcal{E}_i\psi_i, \tag{1}$$

where $V_{\rm ext}(\mathbf{R})$ is the external (pseudo) potential (due to the ion-ion or ion-electron interaction) and $V_{\rm scr}(\mathbf{R})$ is the screening response to such external potentials. The effect of pressure or strain is encoded in the ion-ion geometry underlying $V_{\rm ext}(\mathbf{R})$. The many-particle Hamiltonian is

$$H=\sum_i \mathcal{E}_i^{(e)}c_i^\dagger c_i-\sum_j \mathcal{E}_j^{(h)}h_j^\dagger h_j+\frac{1}{2}\sum_{ijkl}J_{ij;kl}^{(ee)}c_i^\dagger c_j^\dagger c_k c_l + \frac{1}{2}\sum_{ijkl}J_{ij;kl}^{(hh)}h_i^\dagger h_j^\dagger h_k h_l-\frac{1}{2}\sum_{ijkl}[J_{ij;kl}^{(eh)}-K_{ij;kl}^{(eh)}]h_i^\dagger c_j^\dagger c_k h_l, \tag{2}$$

where $c_i^\dagger$ (c_i) and $h_j^\dagger$ (h_j) create (destroy) an electron in the single-particle state $\psi_i^{(e)}$ and a hole in $\psi_j^{(h)}$, respectively. In Eq. (2), the Coulomb and electron-hole exchange matrix elements are given, respectively, by

$$J_{ij;kl}^{(\mu\mu')}=\int\int d\mathbf{R}d\mathbf{R}'\frac{[\psi_i^{(\mu)}(\mathbf{R})]^*[\psi_j^{(\mu')}(\mathbf{R}')]^*[\psi_k^{(\mu')}(\mathbf{R}')][\psi_l^{(\mu)}(\mathbf{R})]}{\epsilon(\mathbf{R},\mathbf{R}')|\mathbf{R}-\mathbf{R}'|}, \tag{3}$$

$$K_{ij;kl}^{(eh)}=\int\int d\mathbf{R}d\mathbf{R}'\frac{[\psi_i^{(h)}(\mathbf{R})]^*[\psi_j^{(e)}(\mathbf{R}')]^*[\psi_k^{(e)}(\mathbf{R})][\psi_l^{(h)}(\mathbf{R}')]}{\epsilon(\mathbf{R},\mathbf{R}')|\mathbf{R}-\mathbf{R}'|}. \tag{4}$$

Here, $\epsilon(\mathbf{R},\mathbf{R}')$ is a phenomenological, microscopic dielectric function that screens the Coulomb and exchange interactions, and in this work we have adopted the $\epsilon(\mathbf{R},\mathbf{R}')$ proposed by Resta.[15] The diagonal elements $J_{ij}^{(\mu\mu')}=J_{ij;ji}^{(\mu\mu')}$ of Eq. (3) are the familiar electron-electron ($\mu\mu'=ee$), hole-hole ($\mu\mu'=hh$), and electron-hole ($\mu\mu'=eh$) direct Coulomb integrals. The electron-electron and hole-hole *exchange* integrals are given by $J_{ij;ij}^{(ee)}$ and $J_{ij;ij}^{(hh)}$, respectively. Solving the single-particle Eq. (1) for a given dot yields the wave functions ψ_i, which are used to construct the Slater determinants $|\Phi(\chi^q)\rangle$ for χ^q and solve the many-particle, configuration-interaction[16] (CI) problem [Eq. (2)]. This gives the total (ground-state) energy $E_{\rm CI}(\chi^q)$ of exciton χ^q, as well as excitonic excited states.

The binding energy of the excitonic complexes are defined as

TABLE I. Comparison of Hartree-Fock (HF) and many-body configuration-interaction (CI) binding energies (in meV), and verification of the "sum rule" $[\Delta_{\mathrm{HF}}(X^-)+\Delta_{\mathrm{HF}}(X^+)]$ for different pressures. For each excitonic complex χ^q, we present the CI binding energy $\Delta_{\mathrm{CI}}(\chi^q)$ as a sum of the Hartree-Fock binding energy $\Delta_{\mathrm{HF}}(\chi^q)$ and correlation-energy component $\delta(\chi^q)=\Delta_{\mathrm{CI}}(\chi^q)-\Delta_{\mathrm{HF}}(\chi^q)$.

Quantity	0.2 GPa	0.8 GPa	1.3 GPa	1.8 GPa	2.4 GPa
$\Delta_{\mathrm{CI}}(X^0)=\Delta_{\mathrm{HF}}(X^0)+\delta(X^0)$	20.8+1.3	21.1+1.4	21.3+1.4	21.6+1.5	21.9+1.5
$\Delta_{\mathrm{CI}}(X^-)=\Delta_{\mathrm{HF}}(X^-)+\delta(X^-)$	1.2+1.3	1.0+1.4	0.8+1.5	0.6+1.6	0.5+1.6
$\Delta_{\mathrm{CI}}(X^+)=\Delta_{\mathrm{HF}}(X^+)+\delta(X^+)$	−1.8+2.4	−1.5+2.3	−1.2+2.3	−0.9+2.2	−0.7+2.2
$\Delta_{\mathrm{CI}}(XX^0)=\Delta_{\mathrm{HF}}(XX^0)+\delta(XX^0)$	−0.6+2.0	−0.4+2.0	−0.3+2.0	−0.3+2.0	−0.2+2.0
$\Delta_{\mathrm{CI}}(X^-)+\Delta_{\mathrm{CI}}(X^+)$	3.1	3.2	3.4	3.5	3.6
Sum rule	−0.6	−0.5	−0.4	−0.3	−0.2

$$\begin{aligned}
\Delta_{\mathrm{CI}}(X^0) &= [\mathcal{E}_0^{(e)} - \mathcal{E}_0^{(h)}] - E_{\mathrm{CI}}(X^0),\\
\Delta_{\mathrm{CI}}(X^-) &= [\mathcal{E}_0^{(e)} + E_{\mathrm{CI}}(X^0)] - E_{\mathrm{CI}}(X^-),\\
\Delta_{\mathrm{CI}}(X^+) &= [-\mathcal{E}_0^{(h)} + E_{\mathrm{CI}}(X^0)] - E_{\mathrm{CI}}(X^+),\\
\Delta_{\mathrm{CI}}(XX^0) &= 2E_{\mathrm{CI}}(X^0) - E_{\mathrm{CI}}(XX^0).
\end{aligned} \tag{5}$$

In a simplified Hartree-Fock (HF) approximation and neglecting the electron-hole exchange $K_{00;00}^{(eh)}$ (which magnitude is of the order of a few to hundreds of μeV),[17] we have

$$\begin{aligned}
\Delta_{\mathrm{HF}}(X^0) &= J_{00}^{(eh)},\\
\Delta_{\mathrm{HF}}(X^-) &= J_{00}^{(eh)} - J_{00}^{(ee)},\\
\Delta_{\mathrm{HF}}(X^+) &= J_{00}^{(eh)} - J_{00}^{(hh)},\\
\Delta_{\mathrm{HF}}(XX^0) &= 2J_{00}^{(eh)} - [J_{00}^{(ee)} + J_{00}^{(hh)}] = \Delta_{\mathrm{HF}}(X^-) + \Delta_{\mathrm{HF}}(X^+).
\end{aligned} \tag{6}$$

The latter relation establishes a "sum rule" for the binding energy of the biexciton at the Hartree-Fock level. The many-body correlation effects $\delta(\chi^q)$ in the binding energy can be quantified by comparing the full solutions in Eq. (5) to the HF ones in Eq. (6),

$$\Delta_{\mathrm{CI}}(\chi^q) = \Delta_{\mathrm{HF}}(\chi^q) + \delta(\chi^q). \tag{7}$$

In this work, we consider a lens-shaped (base diameter $b=252$ Å and height $h=35$ Å) $In_{0.6}Ga_{0.4}As/GaAs$ quantum dot and study how the excitonic binding energies $\Delta_{\mathrm{CI}}(\chi^q)$ depend on pressure (well below the $\Gamma_{1c}-X_{6c}$ crossover).[18] We then analyze this dependence in terms of the pressure dependence of (i) Coulomb integrals $J_{00}^{(\mu\mu')}$ and (ii) correlation energies $\delta(\chi^q)$. In Eq. (1), we use a screened pseudopotential expressed as a superposition of screened atomic pseudopotentials

$$V_{\mathrm{ext}}(\mathbf{R}) + V_{\mathrm{scr}}(\mathbf{R}) = V_{\mathrm{SO}} + \sum_l \sum_\alpha v_\alpha[\mathbf{R} - \mathbf{R}_l^{(\alpha)}; \mathrm{Tr}(\tilde{\varepsilon})], \tag{8}$$

where V_{SO} is a nonlocal spin-orbit pseudopotential;[19] v_α is a screened pseudopotential for an atom of type α that depends on strain; and $\mathbf{R}_l^{(\alpha)}$ is the vector position of atom l of type α after the atomic positions within the simulation supercell (quantum dot+GaAs matrix) have been relaxed, using a valence force field,[19] in order to minimize the elastic energy of the nanostructure. v_α has been fitted to *bulk* properties of GaAs and InAs, including bulk band structures, experimental deformation potentials, and effective masses, as well as local-density approximation (LDA)-determined band offsets.[19] Equation (1) is solved in a basis of linear combination of Bloch bands $\{u_{n\mathbf{k}}^{(M)}(\mathbf{R},\tilde{\varepsilon})\}$ with band index n and wave vector $\mathbf{k}$ of material M(=GaAs,InAs) strained[20] to $\tilde{\varepsilon}$. Thus,

$$\psi_i(\mathbf{R}) = \sum_M \sum_{n,\mathbf{k}} C_{M;n,\mathbf{k}}^{(i)} \left[\frac{1}{\sqrt{N}} u_{n,\mathbf{k}}^{(M)}(\mathbf{R},\tilde{\varepsilon}) e^{i\mathbf{k}\cdot\mathbf{R}}\right], \tag{9}$$

where N is the number of primary cells in the simulation supercell that contains the quantum dot and GaAs matrix. The many-body configuration-interaction expansion is taken over all the Slater determinants $|\Phi(\chi^q)\rangle$ generated within a set of 12 electron and 20 hole single-particle, confined states. Note that in our atomistic approach the pressure affects directly the atomic displacements $\mathbf{R}_i$ and strain $\tilde{\varepsilon}(\mathbf{R})$ and, consequently, the potential $V_{\mathrm{ext}}(\mathbf{R})$ of Eq. (8). As a result, the quantum dot energy levels change as well. In another approach[21] one describes the dot nonatomistically, via bulk-like $\mathbf{k}\cdot\mathbf{p}$ methods. In such a case, one needs to scale the bulk parameters, like effective masses, to the effect of pressure. In our approach effective masses do not enter the formalism.

Direct-Coulomb versus correlation contributions to binding. Table I shows the CI-calculated binding energies $\Delta_{\mathrm{CI}}(\chi^q)$ as well as its decomposition [Eq. (7)] into Hartree-Fock $\Delta_{\mathrm{HF}}(\chi^q)$ and correlation $\delta(\chi^q)$ contributions. We see that (i) the binding energy of the neutral monoexciton X^0 is constituted primarily by HF energy with only 6% being due to correlation. This is in contrast with X^0 in *bulk* semiconductors where $\delta(X^0)$ dominates over $\Delta_{\mathrm{HF}}(X^0)$. (ii) For X^-, X^+, and XX^0 the HF and correlation contributions to binding are comparable. Specifically, while X^- is bound (positive Δ) already in HF, here X^+ and XX^0 are unbound in HF, but become bound by correlation. (iii) For each excitonic complex, the magnitude of the correlations depends weakly on pressure.

Pressure dependence. Figure 1 shows the dependence on pressure of (a) the binding energies $\Delta_{\mathrm{CI}}(\chi^q)$, (b) Coulomb energies $J_{00}^{(ee)}$, $J_{00}^{(eh)}$, and $J_{00}^{(hh)}$, and (c) correlation energies

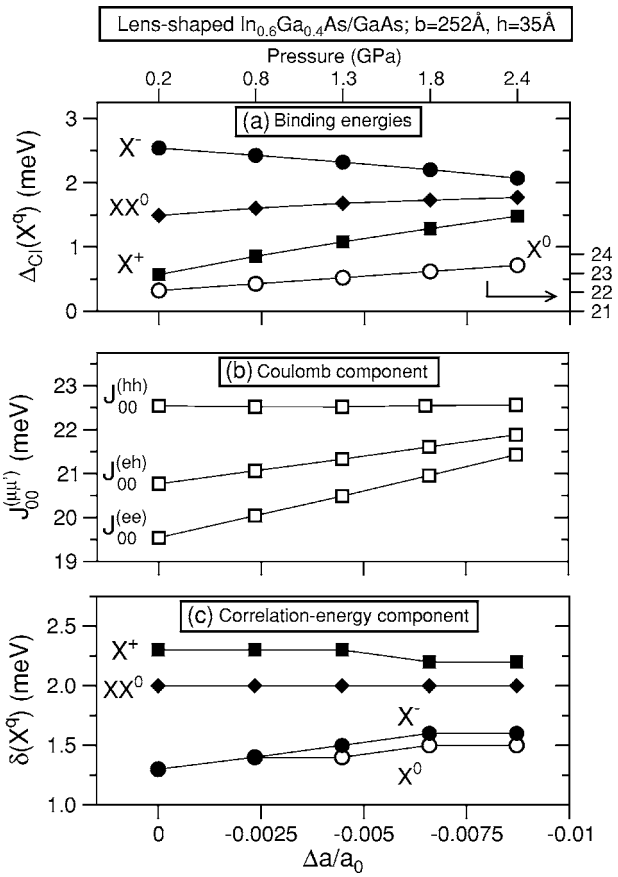

FIG. 1. Pressure dependence of (a) binding energies $\Delta_{CI}(\chi^q)$ as obtained from the many-particle, configuration-interaction method, (b) Coulomb-energy component $J_{00}^{(\mu\mu')}$, and (c) correlation-energy components $\delta(\chi^q)$. (See text for definitions.)

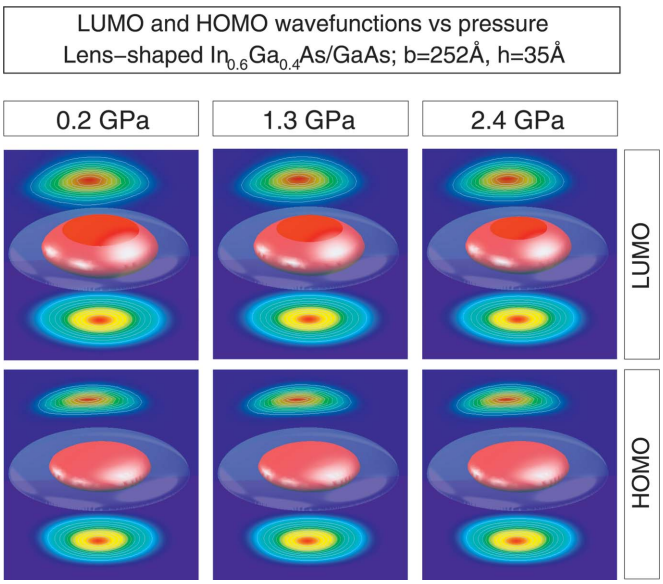

FIG. 2. (Color) LUMO $[\psi_0^{(e)}]$ and HOMO $[\psi_0^{(h)}]$ wave functions at 0.2, 1.3, and 2.4 GPa. The outline of the dot is present as a light shadow. The (red) isosurface encloses 75% of the charge, the in-plane (bottom) contour plot is taken at 1 nm above the dot's base and the out-of-plane contour plot bisects the dot. The LUMO wave function becomes more confined as pressure increases—see the how the wave function penetrates less into the barrier above of the dot as pressure increases; whereas the HOMO wave functions are almost independent of pressure.

$\delta(\chi^q)$. Compression is represented by $\Delta a/a_0=(a-a_0)/a_0$, where a and a_0 are the distorted and equilibrium lattice parameter of the GaAs matrix, respectively. The pressure values showed in the upper axis in Fig. 1(a) are calculated approximately by using the equation of state[22] $P=(B_0/B_0')\times[(V_0/V)^{B_0'}-1]$, where we take $V_0/V=[1+\mathrm{Tr}(\tilde{\varepsilon})]^{-1}$ and calculate $\mathrm{Tr}(\tilde{\varepsilon})$ in the GaAs matrix away from the dot. The calculation of $\tilde{\varepsilon}=\tilde{\varepsilon}(\mathbf{R})$ is performed using atomistic elasticity.[23] We take $B_0=74.7$ GPa and $B_0'=4.67$ as the GaAs bulk modulus and its derivative with respect to pressure, respectively.[24] We see from Fig. 1 that the pressure dependence of the binding energy of the various excitons is different: (i) $\Delta_{CI}(X^0)$ shows a small, nearly linear *increase* with pressure; changing by about 7% in the studied pressure range. $\Delta_{CI}(X^-)$ *decreases* slightly with increasing pressure, while $\Delta_{CI}(X^+)$ *increases* significantly; at $\Delta a/a_0=-0.0087$ ($P=2.4$ GPa) it has increased by 160% compared to its value at $\Delta a/a_0=0$. Similar to the monoexciton case, the binding energy of the biexciton depends only weakly on pressure, showing a small relative change as pressure reaches 2.4 GPa. (ii) Equation (7) shows that the binding has a HF part and a correlation part. Table I showed that the *magnitude* of the binding is decided by the HF part for X^0 and by both HF and correlation for X^-, X^+, and XX^0. However, Fig. 1 shows that the *pressure dependence* is always decided by the HF contribution. (iii) Not surprisingly, the "sum rule" of Eq. (6) valid within HF is not valid at the CI level, quantitatively failing to predict the correct values of the biexciton binding energies. Notwithstanding, the *qualitative* pressure dependence of $\Delta_{CI}(XX^0)$ is reasonably predicted by the "sum rule" at the CI level. (iv) From (ii), we see that the trends of the binding energies with pressure are determined by $J_{00}^{(eh)}$, $J_{00}^{(ee)}$, and $J_{00}^{(hh)}$. By calculating these integrals, we find that $J_{00}^{(hh)}>J_{00}^{(eh)}>J_{00}^{(ee)}$ and the magnitude of $J_{00}^{(eh)}$ and $J_{00}^{(ee)}$ increase with a similar slope as pressure increases while $J_{00}^{(hh)}$ remains nearly constant; see Fig. 1. This explains the decrease of $\Delta_{CI}(X^-)$ and the increase of $\Delta_{CI}(X^+)$ with applied pressure. Further, it also becomes clear why the binding energy of the biexciton remains nearly unchanged with changing pressure: The similar rate of increase of $J_{00}^{(ee)}$ and $J_{00}^{(eh)}$ with pressure combined with the magnitude of $J_{00}^{(hh)}$ leads to a weakly pressure-dependent binding energy for XX^0.

Wave-function localization with pressure. To understand the trend $J_{00}^{(hh)}>J_{00}^{(eh)}>J_{00}^{(ee)}$ and also that $J_{00}^{(hh)}$ has the weakest pressure dependence, while $J_{00}^{(ee)}$ has the strongest, Fig. 2 shows the calculated wave functions for the electron ground state $[\psi_0^{(e)}]$ and hole ground state $[\psi_0^{(h)}]$ as a function of pressure. The isosurfaces enclose 75% of the charge density, the in-plane contour plot is taken at 1 nm above the base of the dot, and the out-of-plane contour plot bisects the dot. We see that the electron is always less localized than the hole. In addition, the electron gets more localized as pressure is applied, while the localization of the hole remains nearly un-

changed. The in-plane (parallel to the base) spatial extension of the electron does not change as much as the out of plane. In particular, Fig. 2 clearly shows that the spatial penetration of the electron wave function into the GaAs matrix decreases with applied pressure. Further, plots (not shown) of the radial charge-accumulation function $\int_0^R d\mathbf{r}|\psi_0^{(s)}(\mathbf{r}+\mathbf{R}_c)|^2$ ($\mathbf{R}_c$ indicates the center of the dot, and the integration is performed over a sphere of radius R; $s=e,h$) for the electron and hole reveal that as pressure increases the electron wave function gets indeed more localized than the hole wave function. The increased localization of the electron with pressure can be explained by the larger magnitude of the conduction-band-edge (CBM) deformation potential of bulk GaAs with respect to that of bulk InAs (Ref. 25), which results in an increased electron confinement in the dot with pressure. In contrast, the similar magnitude of the valence-band-edge (VBM) deformation potential of both bulk GaAs and InAs leads to small changes in hole confinement with pressure and, therefore, to small changes in localization.

Single-particle and excitonic pressure coefficients. We calculate the linear pressure coefficient a by fitting the pressure dependence of the band gap to $E_g(P)=E_g(0)+a\,P+b\,P^2$. For the dot, at the single-particle (SP) level, we obtain $a_{\mathrm{SP}}^{(\mathrm{dot})}=86.47$ meV/GPa, whereas the excitonic value is $a_{\mathrm{CI}}^{(\mathrm{dot})}(X^0)=85.79$ meV/GPa. The latter compares well with the values of 85 meV/GPa (Ref. 8), 80 meV/GPa (Ref. 11), and 82 meV/GPa (Ref. 11) observed in InAs/GaAs dots for the emission lines at 1.28, 1.26, and 1.30 eV, respectively. For bulk GaAs, we obtain $a^{(\mathrm{bulk})}=105.86$ meV/GPa, which is within the range of observed values: 94-120 meV/GPa. (Refs. 18,22). Thus, the dot has a smaller linear pressure coefficient than bulk GaAs. In addition, it is interesting to inspect how the VBM and CBM contribute to the linear pressure coefficient of the band gap. By fitting the lattice-deformation (pressure) dependence of single-particle eigenvalues to $\mathcal{E}_i(a)=\mathcal{E}_i(a_0)+A_i(\Delta a/a_0)+B_i(\Delta a/a_0)^2$, we find $A_{\mathrm{VBM}}^{(\mathrm{dot})}=-1.76$ eV and $A_{\mathrm{CBM}}^{(\mathrm{dot})}=-22.49$ eV. For bulk GaAs we find $A_{\mathrm{VBM}}=-3.74$ eV and $A_{\mathrm{CBM}}=-27.23$ eV. We see that the band-gap response to the lattice distortion (pressure) is largely dominated by the changes in CBM. To reproduce this LDA-predicted[25] behavior, it is necessary to have a pseudopotential that explicitly depends on strain, otherwise one gets $A_{\mathrm{CBM}}=-0.46$ eV and $A_{\mathrm{VBM}}=-11.72$ eV and, consequently, VBM dominates the gap changes.

In summary, we have studied the effects of pressure on the binding energies of X^0, X^-, X^+, and XX^0. Our main findings are the following. (i) With applied pressure, the binding energy of X^0 and X^+ increases and that of X^- decreases, whereas the binding energy of XX^0 is nearly pressure independent. (ii) The correlation-energy component in the binding energy of X^0 is small, whereas it is large in X^-, X^+, and XX^0; indeed, correlation is fully responsible for binding the latter complexes. (iii) Correlations depend weakly on pressure. (iv) The pressure dependence of the binding energies is controlled by the pressure dependence of the direct Coulomb integrals. Further, the relative magnitude (order) of these direct integrals explains the relative magnitude (order) of the binding energies. (v) Pressure dependence of $J_{00}^{(hh)}$, $J_{00}^{(eh)}$, and $J_{00}^{(ee)}$ is explained by the changes of the LUMO and HOMO wave functions with pressure.

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