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We show that a diatomic dot molecule made of two identical, vertically stacked, strained InAs/GaAs $d=9$ nm and as large as 100 n
he few meV found in the large (50–100 nm) electrostatically confined dots.

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Quantum dot molecules (QDM) occupied by two electronic spins have been proposed as a basis for quantum computation.[1] Loss and DiVincenzo[2]

cording to the valence force-field model (VFF) (Refs. 18 and 19). It is clearly seen in Fig. 1(a) that both dots have large and nearly constant hydrostatic strain inside the dots which decays rapidly outside the dots. However, even though the dots comprising the molecule are the same, the strain on the two dots is different since the molecule lacks inversion symmetry. We see that the top dot is slightly more strained than

A microscopic position-dependent dielectric screening[26] is applied to both Coulomb and exchange integrals to represent the inner electrons that are not calculated explicitly. Considering six molecular orbitals $_g$, $_u$, $_u$, $_g$ of Fig. 1(b), we have a total of 66 Slater determinants. The many-body wave functions Ψ are written as linear combinations of these determinants $|\Phi_C\rangle$ as $\Psi = \Sigma_C A\ (C)|\Phi_C\rangle$. The resulting many-particle energies are shown as a function of interdot separation in Fig. 2(b). The energy splittings $J_{S\text{-}T}$ between the ground-state singlet $^1\ ^{(a)}_g$ and triplet ^{3} range from 0–100 meV and are much larger than in electrostatic dot molecules (<1 meV) (Refs. 4–6). In Fig. 3(a) we decompose the two-electron wave functions into the leading configurations $\Phi_1 = |\ \uparrow\ \downarrow\rangle$, $\Phi_2 = |\ \downarrow\ \uparrow\rangle$, $\Phi_3 = |\ \uparrow\ \downarrow\rangle$, and $\Phi_4 = |\ \uparrow\ \downarrow\rangle$. The ground state is the singlet $^1\ ^{(a)}_g$ state, followed by the threefold degenerated triplet states $^3\ _g$ (we depict only the $s_z=0$ state made of $\Phi_1+\Phi_2$ in Fig. 3) and the next singlets $^1\ _u$ (made of $\Phi_1-\Phi_2$) and $^1\ ^{(b)}_g$.

To explore the symmetry breaking of these states, we plot in Figs. 3(b) and 3(c), the pair-correlation functions $P(\ _0,\ ) = |\Psi(\ _0,\ )|^2$ where $_0$ is fixed at the center of the bottom dot. $P(\ _0,\ )$ gives the probability of finding the second electron at position given that the first electron has been found at $_0$. For the ground-state singlet $^1\ ^{(a)}_g$, we see that at the small interdot separation $d=4$ nm, the probability to find the second electron in the top or the bottom dot are comparable, suggesting a molecularlike delocalized state. Accordingly, the wave-function analysis reveals a dominant contribution from the product of two delocalized molecular orbitals Φ_3. By delocalizing into both dots, the electrons can lower their single-particle energy by about 65 meV (about half of the bonding-antibonding splitting), which overcome the Coulomb repulsion between the two electrons. With increasing interdot separation, the electrons show correlation-induced (i.e., the coupling between Φ_3 and Φ_4) localization. At $d=7$ nm, the second electron is almost entirely localized on the top dot as shown in Fig. 3(c). We emphasize that the many-particle wave-function localization is not due to the asymmetry in their single-particle wave functions. This is evident from the fact that in the absence of electron-electron correlations (

with spin , and the other electron is on the l'th orbital of the p' dot with spin ′. The two electrons can be either both on the top dots, or both on the bottom dots, or one on the top and the other on the bottom dots. We can thus define a "bielectron localization parameter" $Q_{pp}^{(\ )}$ as the probability of two electrons occupying the dot $p=(T$ or $B)$