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Correlation, Mott-transition, and singlet-triplet splitting for two electrons in self-assembled InAs/GaAs quantum dot molecules[1] LIXIN HE, GABRIEL BESTER, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, Colorado 80401 — Quantum dot-molecules (QDM) occupied by two electronic spins have been proposed as a basis for quantum computation. Successful operations would require a large singlet-triplet splitting and a low probability of two electrons occupying the same dot. We investigated via atomistic pseudopotential single-particle theory and many-body screened configuration interaction calculations the degree of localization and the magnitude of the singlet-triplet splitting of two electrons in vertically stacked, strained InAs/GaAs self-assembled dots containing $\sim 10^5$ atoms. We find that the ground state is always singlet at all interdot distance and the singlet-triplet splittings are as large as 1 - 100 meV, much larger than these for electrostatically confined dots. The single-particle wavefunctions show symmetry breaking between the top and bottom dots due to the strain effect at inter-dot distance < 4 nm. We find that while the two electrons of the triplet $^3\Sigma$ states show at all interdot distance a correlation-induced Mott-localization of each electron on a different dot, the ground state singlet $^1\Sigma_g$ shows a transition with increasing interdot distance from a molecular state where the two electrons are delocalized over both dots, to a Mott localized state in which each electron is on a different dot.

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