



Excitonic transitions and exchange splitting in Si quantum dots

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$$K_{he,h'e'} = e^2 \sum_{\sigma_1, \sigma_2} \int \int \frac{\psi_{h'}^*(\mathbf{r}_1, \sigma_1) \psi_e^*(\mathbf{r}_2, \sigma_2) \psi_{e'}(\mathbf{r}_1, \sigma_1) \psi_h(\mathbf{r}_2, \sigma_2)}{\bar{v}(|\mathbf{r}_1 - \mathbf{r}_2|, R) |\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2. \quad (5)$$

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The electron–hole Coulomb and exchange integrals of Eqs. (4) and (5) use a screening function  $\bar{v}(\mathbf{r}_1, \mathbf{r}_2, R)$ , which depends on the interparticle distance  $|\mathbf{r}_1 - \mathbf{r}_2|$  and on the quantum dot radius  $R$ . We use the model of Ref. 1 for this screen-

in the single-particle approximation. (ii) When the symmetry of the CBM is  $t_2$ , the direct Coulomb interaction lowers the energy of a dark exciton below the optically active ones. (iii) When the symmetry of the CBM is not  $t_2$ , the lower-energy excitons have  $T_2$  symmetry. (iv) Exchange corrections raise the energy of singlet states. (v) We found that our calculated dark–bright excitonic splitting agrees very well with the experimental optical data of Calcott *et al.*<sup>3</sup> Finally, (vi

pseudopotential wave functions are different from envelope functions, and (b) the dielectric screening  $(r, R)$  entering in  $J$  depends on the size  $R$ . For silicon dots effect (b) is more important than (a), as seen by the fact that using a size-dependent screening with effective mass wave functions gives  $J \sim R^{-1.53}$ . Thus, while simple theory suggests that Coulomb effects tend to become less important as size diminishes, a more accurate calculation shows that Coulomb effects are more important than quantum-confinement effects at small sizes.

In summary, we have found that the electron–hole Coulomb interactions are very important in determining the symmetry of excitons in quantum dots made of a bulk indirect-gap material. In particular, (i) direct Coulomb interactions are able to split the energies of excitons which are degenerate