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Excitonic transitions and exchange splitting in Si quantum dots

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$$K_{he,h'e'}=e^{2}\sum_{\sigma_1,\sigma_2}\int\int\frac{\psi^{*}_{h'}(\mathbf{r}_1,\sigma_1)\,\psi^{*}_{e}(\mathbf{r}_2,\sigma_2)\,\psi_{e'}(\mathbf{r}_1,\sigma_1)\,\psi_{h}(\mathbf{r}_2,\sigma_2)}{\overline{\,}(|\mathbf{r}_1-\mathbf{r}_2|,R)|\mathbf{r}_1-\mathbf{r}_2|}\,d\mathbf{r}_1 d\mathbf{r}_2\,. \tag{5}$$

The electron–hole Coulomb and exchange integrals of Eqs. (4) and (5) use a screening function $\overline{\,}(\mathbf{r}_1,\mathbf{r}_2,R)$, which depends on the interparticle distance $|r_1-r_2|$ and on the quantum dot radius R. We use the model of Ref. 1 for this screenpseudopotential 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 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.*[3] Finally, (vi