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Quasiparticle Gaps and Exciton Coulomb Energies in Si Nanoshells KIMBERLY FREY, JUAN C. IDROBO, SERDAR OGUT[1], University of Illinois at Chicago, MURILO L. TIAGO, FERNANDO A. REBOREDO[2], Oak Ridge National Laboratory — Quasiparticle gaps and exciton Coulomb energies are calculated in Si nanoshells passivated by H at the inner and outer surfaces. We consider spherical nanoshells with inner radii R_1 up to 1 nm and outer radii R_2 up to 1.6 nm. Quasiparticle gaps are calculated using ΔSCF and GW methods. While the single-band effective mass approximation predicts that the gap should depend only on the thickness $t = R_2 - R_1$ of the nanoshell, we find from first principles calculations that it depends on both R_1 and R_2. The dependences of the quasiparticle gap on R_1 and R_2 are mostly consistent with electrostatics of a charged metallic shell. We also find that the (unscreened) Coulomb energy in Si nanoshells has a somewhat unexpected size dependence at fixed outer radius R_2. Namely, the exciton Coulomb energy *decreases* as the nanoshell becomes more *confining*, contrary to what one would expect from quantum confinement effects. We show that this is a consequence of an increase in the average electron-hole distance, giving rise to reduced exciton Coulomb energies in spite of the reduction in the confining nanoshell volume.

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