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Density functional theory studies of core-shell semiconductor nanoparticle quantum dots BRENT WALKER, SHAUN HENDY, Industrial Research Limited, 69 Gracefield Road, P.O. Box 31-310, Lower Hutt 5040, New Zealand, RICHARD TILLEY, School of Chemical and Physical Sciences, Victoria University of Wellington, P. O. Box 600, Wellington, New Zealand — In going from the macroscale to the nanoscale, quantum-mechanical effects become increasingly important and may mean that nanostructures of a material exhibit very different properties from the corresponding bulk. This is especially noticeable in the case of the optical properties of semiconductor nanoparticles (or quantum dots), which display a number of remarkable features (including very distinct peaks, and tunability across a broad range of wavelengths), due to quantum confinement. Our work involves modeling Si-Ge core-shell nanoparticles using large-scale computer simulations based on the density functional and time-dependent density functional theories. These simulations in particular provide us with predictions of the geometric structures and optical absorption spectra of nanoparticles in an accurate and computationally efficient way, and allow us to study the systematic trends in these properties as the composition and size of the nanoparticle change.

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