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***Ab-initio* studies of semiconductor quantum dots** BRENT WALKER, SHAUN HENDY, Industrial Research Ltd, PO Box 31-310, Gracefield Rd, Lower Hutt, New Zealand, RICHARD TILLEY, School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand — Quantum dots (QDs) in the form of semiconductor nanocrystals have considerable potential as cell markers/disease trackers in medical physics due to their favorable light-emitting properties and long lifetimes in the cellular environment. Quantum confinement is believed to be responsible for the optical properties of semiconductor QDs (for instance, the direct band gap transition in H or C terminated Si dots is allowed); size and surface functionalization both affect the degree of quantum confinement in the QD, and hence its electronic and optical properties. We present *ab-initio* computational studies of Si and Ge based nanocrystals made using density functional theory (DFT); in particular, we obtain optical absorption spectra by application of Lanczos algorithms to the central equations of linear-response time-dependent DFT [1]. We examine how the atomic geometries, electronic structure and optical absorption spectra are affected by the nanocrystal size and surface functionalization. [1] B. Walker, A. M. Saitta, R. Gebauer, and S. Baroni, *Phys. Rev. Lett.*, **96**, 113001, (2006).

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