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Symmetry considerations for semiconductor nanocrystals GUSTAVO M. DALPIAN, University of Texas, MURILO L. TIAGO, MARIE LOPEZ DEL PUERTO, University of Minnesota, JAMES R. CHELIKOWSKY, University of Texas — Semiconductor nanocrystals or quantum dots show a wide range of physical properties with respect to their size or shape. In this paper we show that symmetry is also an important characteristic that can lead to different electronic and optical properties, mainly for small nanocrystals. This means that two spherical nanocrystals with similar sizes but different symmetries have different optical and electronic signatures, which should be accessible experimentally. We use pseudopotential density- functional theory, on a real space approach, to address the differences between spherical nanocrystals with similar sizes but different symmetries. We will report differences in the energy gap, the crystal field splitting and the absorption spectra for CdSe nanocrystals. The symmetry of the nanocrystal is also important when studying doping of nanocrystals.

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