

Abstract Submitted  
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**Discrete size series of CdSe quantum dots: A combined computational and experimental investigation** MIN YU, GAYANATH FERNANDO, RONGFU LI, FOTIOS PAPADIMITRAKOPOULOS, NING SHI, RAMAMURTHY RAMPRASAD — Ab initio computational studies were performed for CdSe nanocrystals over a wide range of sizes in conjunction with recent experimental work. Substantial relaxations and coordination of surface atoms were found to play a crucial role in determining the nanocrystal stability and optical properties. While optimally (three-fold) coordinated surface atoms resulted in stable closed-shell structures with large optical gaps, sub-optimal coordination gave rise to lower stability and negligible optical gaps. These computations are in qualitative agreement with recent chemical etching experiments suggesting that closed shell nanocrystals contribute strongly to photoluminescence quantum yield while clusters with non-optimal surface coordination do not.

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