Abstract Submitted
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First-Principles Calculations of Lattice-Strained Core-Shell Nanocrystals[1] K.H. KHOO, Institute of High Performance Computing, A*STAR, J.T. ARANTES, Universidade Federal do ABC, JAMES R. CHELIKOWSKY, University of Texas at Austin, G.M. DALPIAN, Universidade Federal do ABC — We have studied the properties of CdS-ZnS and ZnS-CdS core-shell nanocrystals over a range of shell thicknesses using real-space pseudopotential density functional theory. The effect of structural relaxation was shown to be important as it leads to significant changes in the HOMO-LUMO gap and frontier orbital localizations. Also, strains due to lattice mismatch are predicted to be highly localized around the core-shell interface, giving rise to a thin shell regime where both confinement and strain effects are important and a thick shell regime where confinement effects dominate. This has interesting implications for the evolution of the HOMO-LUMO gap with shell thickness.

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