Abstract Submitted
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First Principles Study of Core-Shell Semiconductor Nanocrystals[1] IGOR VASILIEV, New Mexico State University — Core-shell nanocrystals composed of two different semiconductors have recently attracted considerable attention. These structures provide enhanced functionality and possess more degrees of freedom than single-component semiconductor nanocrystals and quantum dots. I present the results of *ab initio* density functional calculations for the structures, electronic densities of states, and optical absorption gaps of core-shell nanocrystals composed of group II-VI semiconductors, such as CdSe, CdTe, ZnSe, and ZnTe. The outer surfaces of the nanocrystals are passivated using partially charged hydrogen atoms. The calculations are performed for "traditional" core-shell nanocrystals, in which a core a narrow gap semiconductor is covered with a shell of a wide gap material, and "inverted" core-shell nanocrystals, in which a wide-gap core is enclosed in a narrow-gap shell.

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