

Abstract Submitted
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Geometries of small cadmium selenide clusters¹ MOHAN VARANASI, MICHAEL LISOWSKI, RONALD COSBY, Ball State University — The sizes, shapes, relaxed atomic positions, eigenvalues, and total energies are calculated for selected ultrasmall CdSe clusters using SIESTA, a software package for electronic structure calculations and molecular dynamics simulations of molecules and solids. The properties of these bare clusters with small numbers of constituent atoms are studied using density functional theory (DFT) for energy calculations and the conjugate gradient approximation method in relaxing the structure to find the lowest energy configurations. The *ab-initio* norm-conserving pseudopotentials, the exchange-correlation approximation, and parameters used in the computations are discussed. We describe ancillary software for calculating initial atomic coordinates, testing pseudopotential transferability, and conveniently generating input data files.

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