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InP Nanocrystals Core and Surface Electronic Structure from Ab Initio Calculations

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Abstract : The ab initio restricted Hartree-Fock method is used to simulate the electronic structure of indium phosphide (InP) nanocrystals (NCs) (216-738 atoms) with sizes ranging up to about 2.5 nm in diameter. The calculations are divided into two parts, surface, and core. The oxygenated (001)-(1×1) facet that expands with larger sizes of nanocrystals is investigated to determine the rule of the surface in nanocrystals electronic structure. Results show that lattice constant and ionicity of the core part show decreasing order as nanocrystals grow up in size. The smallest investigated nanocrystal is 1.6% larger in lattice constant and 131.05% larger in ionicity than the converged value of largest investigated nanocrystal. Increasing nanocrystals size also resulted in an increase of core cohesive energy (absolute value), increase of core energy gap, and increase of core valence. The surface states are found mostly non-degenerated because of the effect of surface discontinuity and oxygen atoms. Valence bandwidth is wider on the surface due to splitting and oxygen atoms. The method also shows fluctuations in the converged energy gap, valence bandwidth and cohesive energy of core part of nanocrystals duo to shape variation. The present work suggests the addition of ionicity and lattice constant to the quantities that are affected by quantum confinement phenomenon. The method of the present model has threefold results; it can be used to approach the electronic structure of crystals bulk, surface, and nanocrystals.

Keywords : InP, nanocrystals core, ionicity, Hartree-Fock method, large unit cell
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