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Effect of effective mass and spontaneous polarization on photocatalytic activity of wurtzite and zinc-blende ZnS

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Abstract

Semiconductor zinc sulphide (ZnS) has two common phases: hexagonal wurtzite and cubic zinc-blende structures. The crystal structures, energy band structures, density of states (DOS), bond populations, and optical properties of wurtzite and zinc-blende ZnS were investigated by the density functional theory of first-principles. The similar band gaps and DOS of wurtzite and zinc-blende ZnS were found and implied the similarities in crystal structures. However, the distortion of ZnS4 tetrahedron in wurtzite ZnS resulted in the production of spontaneous polarization and internal electric field, which was beneficial for the transfer and separation of photogenerated electrons and holes. (C) 2015 Author(s).

Keywords

KeyWords Plus: HYDROGEN-PRODUCTION; ANATASE TiO2; WATER; NANOPARTICLES; CONDUCTION; SURFACE; SEMICONDUCTORS; NANOCOMPOSITE; DECOMPOSITION; COMPLEXES

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