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SI/LATIO₃ SEMICONDUCTOR-OXIDE INTERPHASE: A DFT THEORETICAL STUDY

LaTiO₃ (LTO) perovskite is a Mott-Hubbard insulator; however, its electronic and magnetic properties can be modulated by substitutional defects, quantum confinement or heterojunction with a semiconductor material such as Si. For this work, these effects were investigated using density functional theory (DFT). The model used consisted of cutting a slab from the LTO bulk phase so that the system is two-dimensionally (2D) confined, the free surfaces are parallel to the (001) crystallographic planes and have a TiO₂ termination. Then, to form a Si monolayer on the LTO slab, Si atoms were placed at highly symmetric absorption sites as follows: top sites for Ti and O atoms and hollow sites in the center of the ring formed by O and Ti atoms. Another nanostructured model was created by substituting La with Li atoms in the LTO bulk phase. Similar to the Li-free case, this forms a 2D confined perovskite system; in addition, Si atoms were positioned at the aforementioned absorption sites. Results shown that the electronic and magnetic properties of each system notoriously depend on the confinement and the substitutional Li defects. For all cases, Si atoms interact strongly with O and Ti atoms; this fact was evidenced by means of the electronic density difference analysis and there are suggestions of covalent and ionic Si-Ti and Si-O bonds, respectively.

Keywords

Li-batteries, DFT, nanostructured systems, perovskites

Reference

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