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Band-gap engineering of SnO_2

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ABSTRACT

Using first principles calculations based on density functional theory (DFT), the electronic properties of SnO_2 bulk and thin films are studied. The electronic band structures and total energy over a range of SnO_2-multilayer have been studied using DFT within the local density approximation (LDA). We show that changing the interatomic distances and relative positions of atoms could modify the band-gap energy of SnO_2 semiconductors. Electronic-structure calculations show that band-gap engineering is a powerful technique for the design of new promising candidates with a direct band-gap. Our results present an important advancement toward controlling the band structure and optoelectronic properties of few-layer SnO_2 via strain engineering, with important implications for practical device applications.

1. Introduction

Semiconductor nanomaterials, as the significant foundations for various nanoscale electronic and optoelectronic devices, such as single-electron transistors, single-molecule sensors, and nanowire lasers, have attracted a great deal of attention [1–7]. The tin oxide semiconductor nanomaterials are of great industrial interest due to their unique properties, such as the n-type semiconductor character, the high optical transmission in the visible range, the infrared reflection, transparent thermal barrier component, and good chemical stability. They are also used in the design of chemical sensors [8–11]. However, the physicochemical properties of these semiconductors are closely related to the procedures and conditions for their development. Indeed, it will be possible to obtain films having a crystalline or amorphous structure according to the methods of their fabrication; their structural properties are then affected. These play an important role in the optical and electrical properties of the layers. They also influence on their chemical stability in time. Problems related to these deposits can come either from the technology itself or compounds used as precursors or even synthetic conditions. All of these parameters have a major impact on the structural properties (grain size, aggregate size), optical (layer thickness, refractive index, absorption, reflection and transmission in different regions of the electromagnetic spectrum) and electric (electrical conductivity, carrier density, and quantum confinement) of the oxide formed [12–14]. Among the transparent conductive oxide (TCO) materials, tin dioxide (SnO_2) has gained extensive attention of researchers over the past decades owing to its excellent electrical, optical, and electro-chemical properties, which is also attractive for potential applications such as solar cells and flat panel displays. However, bulk SnO_2 cannot efficiently emit UV light due to the dipole forbidden nature of its band edge quantum states, which has hindered its potential optoelectronic applications. Most studies reported a dominant broad visible emission band centered at around 540 nm instead of the near band edge (NBE) UV emission for bulk SnO_2. To recover the optical activity of SnO_2 corresponding to the “forbidden” band gap, and to use it as a UV light emitter, some researchers attempted to utilize SnO_2 nanostructures, including nanowires and quantum dots, to modify SnO_2 electronic structure so that the dipole forbidden rule can be broken. The study of these materials, in thin and ultra thin layers, is motivated by the need to integrate these materials in miniaturized devices as well as the study of new phenomena occurring at the nanoscale. However, to our knowledge, the compressive investigations of these materials in thin and ultra thin layers are still lacking in the experimental and theoretical reports. Therefore, we will study the structural, electronic, and optical properties of thin layers and ultra thin SnO_2. In this way, the main goal of this work is to study

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the effect of layer thickness, and the evaluation of the structural and optical properties, as well as their electronic structure properties. The electronic structure and band structure properties of semiconductors have been improved, by the effect of external pressure and internal strain via the interatomic distances and relative positions of atoms.

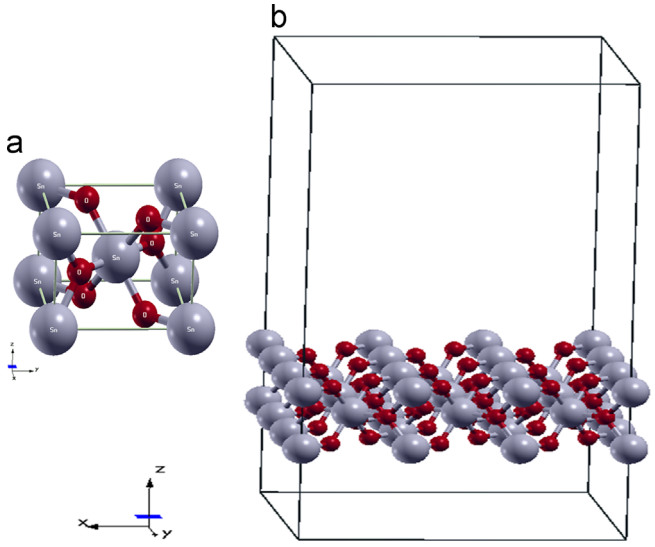

Fig. 1. Optimized stable (a) unit cell and (b) 1 layer of SnO_2.

2. Computational details

To solve the density functional theory (DFT) one-particle equations, we use a multiple-scattering theory, i.e. the KKR Green's function method combined with the coherent potential approximation (CPA). The relativistic effects have been taken into account by employing the scalar relativistic approximation. The form of the crystal potential has been approximated by a muffin-tin potential, and the wave functions in the respective muffin-tin spheres have been expanded in real harmonics up to "$l=2$", where "l" is the angular momentum quantum number defined at each site. In the present KKR-CPA calculations, where the package MACHIKANEYAMA2000 coded by Akai [15] is used, 500 K-points in the whole first Brillouin zone were taken into account. In this study, the KKR method within the Local Density Approximation (LDA) has been used for the parameterization of the exchange energy [16]. The SnO_2 oxide crystallizes in the rutile-type structure (P42/mnm, space group No. 136) at ambient conditions. The Wyckoff position of Sn and O are $2a$ (0,0,0) and $4f$ (u,u,0), respectively, where $u=0.3056$ [17]. In order to achieve a good packing, 8 additional "empty" spheres (ES) with ($Z=0$) representing atomic inter-sites are placed in (½,0,0.1682), (0,½,−0.1682), (0,½,0.1682), (½,0,0.1682), (−0.3125,0.3125,0), (−0.1875,−0.1875,0), (0.1875,0.1875, 0), and (0.3125,−0.3125,0). The lattice constants used as input in the calculation are the experimental values [17]. For SnO_2 thin and ultra thin layers are constructed from 3D rutile structure. All structures were treated with periodic boundary conditions in the x-, y-direction to simulate an infinite plane, and the supercell was large enough to ensure a vacuum spacing along the z-direction to get 2, 4 and 8 layers.

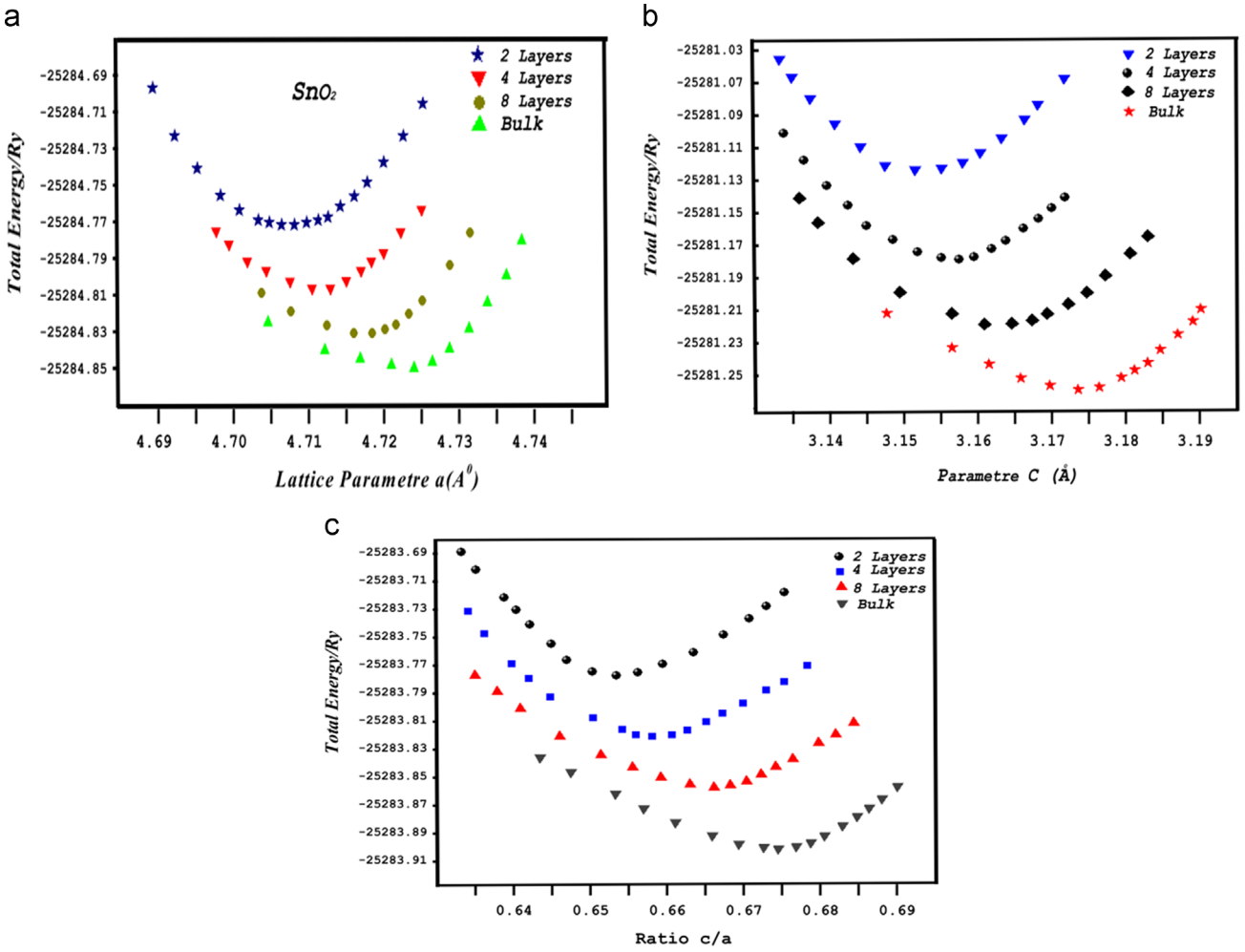

Fig. 2. First-principles calculation of total energy versus lattice parameter of SnO_2 multilayer compared to the bulk system.