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A Study Focused on Ab-Initio Study of $SrTiO_3$ Perovskites

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Abstract: ***ABO_3-type perovskite crystals are important for numerous technological applications in electro optics, waveguides, laser frequency doubling, high capacity computer memory cells, etc.. The perovskite-type materials have been under intensive investigation at least for half a century, but, from theoretical point of view, a proper description of their electronic properties is still an area of active research. The $SrTiO_3$ perovskites has attracted considerable attention in the last years because it is interesting semiconductor materials with active optical properties such as electroluminescence and photoluminescence (PL) at low temperature and thus may be used as new optoelectronic devices with superior performance. Due to its high technological interestSrTio$_3$ perovskites are also the focus of numerous theoretical–computational studies. The $SrTiO_3$ is classical representatives of perovskites belonging to the $A^{II}B^{IV}O_3$ group. So the present Ab- Initio study is plan to evaluate the different parameters of $SrTiO_3$.***

Keywords: ABO_3-type perovskite, $SrTiO_3$, $A^{II}B^{IV}O_3$ group, electroluminescence

1. Introduction

The availability of enormous developments in computer technology made computational material science to appear as a new interdisciplinary branch of science and technology to study such types of materials. Yet, it would not be this much successful without modern density functional theory (DFT).

The complex crystalline systems containing many atoms can be studied using computer simulations. There are different methods ranging from classical to quantum mechanical (QM) approaches to perform such simulations. The classical approach are force field or semi-empirical schemes, in which the forces that determine the interactions between the atoms are parameterized in order to reproduce a series of experimental data, such as equilibrium geometries, bulk muduli or lattice vibrational frequencies. These schemes are often useful within a given class of materials provided good parameters are already known. If, however, such parameters are not available, or if a system shows unusual phenomena that are not yet understood, one must rely only on *ab initio* calculations. They are more demanding in terms of computer requirements and thus allow only the treatment of much smaller unit cells than semi-empirical calculations do. The advantage of first-principle methods lies in the fact that they do not require any experimental knowledge to carry out such calculations. There are two types of approaches for a full quantum mechanical treatment: HF and DFT. The traditional scheme is the HF method which is based on a wave function in a form of one Slater determinant. Exchange is treated exactly but correlation effects are neglected. The latter can be included by more sophisticated approaches. An alternative scheme is DFT which is commonly used to calculate the electronic structure of complex systems containing many atoms such as large molecules or solids. It is based on the electron density rather than on the wave functions and treats both exchange and correlation, but both approximately. It has offered new possibilities to design novel materials and devices by giving precise quantitative physical predictions.

ABINIT is a package whose main program allows finding the total energy, charge density and electronic structure of systems made of electrons and nuclei within density functional theory, using pseudopotentials and a planewave basis. ABINIT is not the fastest code around, but it is one of the best featured and best maintained. The number of different features implemented is greater than any other code.

Abbreviations

1. **DFT- Density functional theory**
2. **ABINIT- A software**
3. **HF- Haretree- Fock Method**

2. Methodology

(a) In computation of total energy of transition metal perovskites, we will use planewave and pseudopotentials. ABINIT program admits many different types of pseudopotentials e.g. Troullier-Martins type, Goedecker type etc. which will be used suitably. The total free energy will be calculated for $SrTiO_3$ perovskites by providing corresponding input variables. The different components of energy will be computed and the results will be analyzed and compared with the available experimental results.

(b) The computation of charge densities of above titanates perovskites will be done by choosing the appropriate variables and the analysis will be done using post-processor called “Cut 3D”. It can analyze the charge contained in an atomic sphere and perform the Hirshfeld computation of atomic charges. In order to visualize the charge density contours we will use MATLAB.

(c) Numerical calculation of forces, stresses and their decomposition into different components will be done. By proper choice of cut-off energies and grid of k-points lattice parameters for the perovskites will be calculated and results will be compared with other available experimental or theoretical results.

(d) Computation of band structure will be done by solving the Kohn-Sham equation for many different k-points, along different lines of the Brillouin zone. The potential that enters the Kohn-Sham will be derived from a previous self-consistent calculation. We will use MATLAB as a graphical tool for representation of band structure. Analysis and limitations of structure will be discussed and improvements will be suggested.

3. Discussion

The electronic structure of perovskites has been recently calculated from first principles and published by several research groups. One of the first theoretical investigations of the ferroelectric transitions in BTO and PTO perovskite crystals have been performed by Cohen and Krakauer in the beginning of 90s [1-3]. Authors used the all-electron full-potential linearized augmented-plane-wave method within the local density approximation (LDA). In 1994 the systematic study of structural and dynamical properties for eight various perovskites has been published by King-Smith and Vanderbilt [4]. They used the ultrasoft-pseudopotential method and the LDA. A few years later Tinte and Stachiotti [5] reported the results of local spin density approximation and Perdew–Burke–Erzernhof generelaized gradient approximation (GGA) calculations for above-mentioned properties of four perovskite oxides. Most recently, Cora and Catlow examined the electronic structure of a wide range of perovskites using ab initio HF method [6]. Also, the detailed description of the atomic and electronic properties of PTO can be found in studies performed by Ghosez, Waghmare and co-workers [7,8], and Cappellini et al. who applied a perturbative approximation, based on a set of selfconsistent equations for the one-electron Green_s function involving a screened potential, to the calculations of ground-state properties of STO and related binary ionic oxides, SrO and MgO [9]. All these studies show the considerable progress in calculations of various perovskite properties.

Perovskites $SrMO_3$ attracts much attention from physicists and material scientists because of the unusual combination of their magnetic, electronic and transport properties [10-15]. However the electronic structure features in these complicated systems are not understood comprehensively yet and attempts to explain their behavior in different conditions are often based on oversimplified models. Though quite a number of publications are known on strontium oxide perovskites with 3d metals on M-sites [16-19] the main focus of the research is $SrTiO_3$-one of the generic representative of transition metal perovskites.

The surface relaxation and rumpling have been experimentally studied by means of low-energy electron diffraction, high energy electron diffraction, medium energy ion scattering & surface X-ray diffraction measurements [20-25]. Bulk properties and electronic structure of SrTiO3, BaTiO3,PbTiO3 perovskites: an ab initio HF/DFT study was done by S. Piskunov ,, E. Heifets , R.I. Eglitis , G. Borstel [26].

The first ab initio calculations of the $SrTiO_3$ surface was performed by Bottin et al., [30] who carried out a systematic first-principles study of the electronic and atomic structure of several (1x1) terminations of the (011) surface. The electronic structures of the stoichiometric SrTiO and O_2 terminations were characterized by marked differences with respect to the bulk, as a consequence of the polarity compensation. One year later, Heifets et al. [31] performed ab-initio Hartree-Fock calculations for four possible terminations (TiO, Sr, and two kinds of O terminations) of the $SrTiO_3$ surface. Finally, Eglitis and Vanderbilt [32] performed ab initio calculations for the technologically important $BaTiO_3$ and $PbTiO_3$ surfaces.

Some attention was given to related materials like perovskite $SrVO_3$, solid solutions $SrTi_{1-x}V_xO_3$, $SrVO_3/SrTiO_3$ superlattices and heteroepitaxial structures $SrVO_3/SrTiO_3/Si$ [33, 34]. H. Kunpyo proposed a model that involved localized states or bands to explain the properties of compounds in the solid solution of $SrTi_{1-x}V_xO_3$ [35]. S.M.Jaya et al. performed electronic structure calculations of the perovskite oxides $SrFeO_3$ & $SrCoO_3$ using self-consistent linear muffin-tin orbital method [36]. Using their optical conductivity spectra Lee et al. investigated the electronic structures of the perovskite-type 4d transition metal oxides [37]. Theoretical studies of surfaces of these oxides have been numerous. On the experimental side the study of such surfaces is complicated due to presence of surface defects. Wolfram and coauthors [38] using a linear combination of atomic orbital approach, predicted mid-gap surface for $SrTiO_3$, in disagreement with experimental investigations [39, 40]. Many more scientists used various approaches to study these surfaces [41, 42, 43]. Quantum and classical modeling of the water adsorption on the surfaces of $SrMO_3$ (M = Ti, Zr, Hf) has been performed and possibility of the water molecule dissociation was investigated at Department of Quantum Chemistry, St. Petersburg by Evares tov et al. [44]. Nevrasov presented parameter-free LDA+DMFT results for the many body spectra of cubic $SrVO_3$ and orthorhombic $CaVO_3$ [45].

Recently a comparative study of the electronic structures of $SrMO_3$ (M = Ti, V, Mn, Fe, Co; M = Zr, Mo, Ru, Rh) by O 1 S X-ray absorption spectroscopy was done by Han-Jin Noh and coauthors [46]. First-principles calculation of the phase transition in CaTiO3 under negative static pressure was performed to examine in detail the phase relationships in these systems by Moriwake et al. [47]. Ab initio calculations of phonon spectra in ATiO3 perovskite crystals (A = Ca, Sr, Ba, Ra, Cd, Zn, Mg, Ge, Sn, Pb) was carried out by Alexander I. Lebedev [48].

4. Conclusion

The band structure, total energy, lattice parameters, and charge density of some $SrTiO_3$ perovskites is calculated by the help of ABINIT software. The basic conclusions are compared with experimental results of different parameters of pseudopotential method based on density functional theory in the local density approximation (LDA) and in generalized gradient approximation (GGA). Plane waves are used as a basis set for the electronic wave functions in the solution of Kohn-Sham equation. By using main ABINIT code along with different utility programs, the results found useful in transition metal perovskites.

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