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Title :
AB-Initio Studies on Properties of Strain-Free and Strained Perovskite-Type (ABO₃) Multiferroic Materials

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Multiferroic is one of the potential multifunctional materials for applications in novel based devices including magnetoelectric memory, spintronic and sensor. Efforts to develop more efficient multiferroic materials provide new opportunities and challenges in this field. Existing multiferroic materials were modified to enhance their existing properties. One of the known multiferroic materials is BiFeO₃ which has a great potential to exhibit excellent multiferroic properties at room temperature. In this work, the investigation focuses on the variety functional and physical properties of strain-free and strained perovskite-type multiferroic materials. The ab-initio calculations based on Density Functional Theory plus on-site Coulomb repulsion U method (LDA+U and GGA-PBEsol+U) as implemented in plane-wave pseudopotential CASTEP code were employed. The structural, lower energy symmetry, electronic, optical and elastic properties of strain-free BiFeO₃ were preliminary determined. It has been shown that the application of self-interaction corrected LDA+U and GGA-PBEsol+U functionals improve the accuracy of calculated properties. The results of structural, electronic, elastic and optical properties of BiFeO₃, calculated

using LDA+U and GGA-PBEsol+U are in good agreement with other available calculations and experimental data. The lower energy symmetry of strained BiFeO₃ was then studied via ab-initio calculation. The calculation revealed that the possible structural phase transformation discovered in strained BiFeO₃ is due to the difference in volumetric strain effects. Moreover, misfit strain effects on the structural phase transformation, morphotropic phase boundary and physical properties of epitaxial BiFeO₃ thin film were further investigated. The major finding in this study reveals that the coexistence of rhombohedral-like and tetragonal-like phases in epitaxial BiFeO₃ thin film occurred at moderate compressive strain of in-plane a-lattice parameter, which is also in excellent agreement with recent experimental studies. The optical blue shifted in monoclinic phase and red shifted impure tetragonal phase of epitaxial BiFeO₃ thin film were also discovered. Additionally, the modified BiFeO₃ was investigated by substituting the Bi (III) with La (III). The rhombohedral to orthorhombic phase transformation in Bi_{1-x}La_xFeO₃ solid solution was determined at x= 0.57 for rhombohedral *R3c* and orthorhombic *P21a* phases respectively, which are consistent with available experimental and other calculation studies. Furthermore, the novel perovskite-type materials based on lone pair SbFeO₃ and BiVO₃ compounds were successfully designed in this work using ab-initio computational method. It has been found that the most stable crystal structure of SbFeO₃ is antiferromagnetic monoclinic *Pc* phase. For BiVO₃, ferromagnetic monoclinic *P21/a* phase (LaVO₃-like structure) is found to be the most stable structure. These novel compounds have been found to demonstrate the structural phase transformation to polar monoclinic *Pm* and *Cc* phases under expansive volumetric strain effects. It is noted that the BiVO₃ and SbFeO₃ are metastable phase compounds under strain effect, which may be possible to be produced from high pressure-high temperature synthesis and epitaxial thin film growth techniques. Thus, the advanced epitaxial thin film growth technique is suggested as a potential method to synthesize BiVO₃ and SbFeO₃ single phase, which are promising candidates to be novel multiferroic materials.