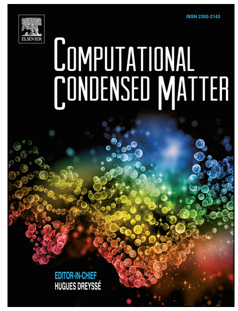

Enhancement of piezoelectricity of tetragonal P4mm $SrHfO_3$ under uniaxial stress: A first principle study

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Enhancement of piezoelectricity of tetragonal P4mm $SrHfO_3$ under uniaxial stress: A first principle study

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Abstract

First principle calculations in the framework of density functional theory and density functional perturbation theory within the generalized gradient approximation are used to calculate the ground state polarization, Born effective charges and piezoelectric strain constant d_{33} of hypothetical tetragonal P4mm $SrHfO_3$. Our results predict the occurrence of piezoelectricity in this hypothetical system. Born effective charges of both Hf and O atoms are much larger than their anticipated nominal charges which show a strong hybridization between Hf and O atomic orbitals. The effect of uniaxial stress along the c-axis on polarization, Born effective charges and piezoelectric strain coefficient d_{33} are also studied. We found that the polarization will increase as the uniaxial stress raises from negative to positive values. These changes suggest that the uniaxial tensile stress could raise the ferroelectricity, while the uniaxial compressive stress would cancel it. We also found that the piezoelectricity of this system could be improved by applying stress. These results could be significant in the field of lead free piezoelectric materials.

Keywords: density functional perturbation theory, piezoelectricity, lead free piezoelectric material, Born effective charges

Introduction

Piezoelectric materials that can generate electricity in response to an external mechanical stress or vice versa, are the main operating part of acoustic and ultrasonic transducers, sensors, ultrasonic imaging devices, hydrophones and many other smart devices in modern world [1-4]. Among different kinds of piezoelectric materials, lead zirconate titanate $PbZr_{(1-x)}Ti_xO_3$ (PZT) is the most widely investigated and used piezoelectric ceramic because of its low cost and high piezoelectric properties [5, 6]. Since PZTs contain significant amounts of toxic lead they are not environmental friendly and it is necessary to look for an appropriate substitute for it. Therefore studies on lead free piezoelectric materials have attracted much attention in recent years [7, 8]. Some of the lead free piezoelectric materials that have been studied are systems based on bismuth sodium titanate (BNT), bismuth potassium titanate (BKT), potassium sodium niobate (PNN) etc [7, 9]. Unfortunately these systems have low piezoelectric properties. However, systems with higher piezoelectric characteristics have been developed such as barium zirconate titanate-barium calcium titanate (BZT-BCT) [10, 11]. Despite extensive investigations which have been conducted on lead free materials, the practical application of these materials is not in a proper situation. Thus any theoretical and experimental attempt to find new lead free material with high piezoelectric properties is valuable [7].