Ferroelectricity of $CsRbPb_2I_6$ superlattice

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ANM-nanomaterial-Poster

INTRODUCTION

$MAPbI_3$ perovskites has been considered as promising material for low-cost, high-efficiency solar cells[1] Many studies have followed with the aim of investigation the fundamental properties of perovskites. Theoretical calculations suggested the possibility of ferroelectricity of $MAPbI_3$[2].

THEORETICAL STUDY

In this study, we have performed ab-initio calculations of $CsRbPb_2I_6$ halyde perovskites. Used approach is density functional calculations with the PBE-GGA[3]. The momentum space integrations were performed using a $5 \times 4 \times 4$ Γ-centered Monkhorst-Pack k-mesh[4]. We have applied a linearized form of the investigation of total polarization of a crystal. This method combines Berry Phase born effective charges and displacements of ions from ideal positions[5].

RESULTS AND DISCUSSION

The unit cell of perovskite contains 20 atoms. Space group of [001] layered supercell is $Pmc2_1$, [111] rocksalt supercell`s space group is $Pna2_1$, this is actually a polar space groups shown in Fig. 1.

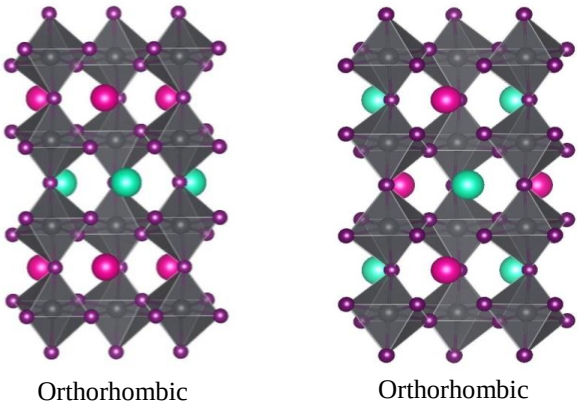

Figure 1. Structure of $CsRbPb_2I_6$ superlattices in [001] and [111] directions[6]

The value of spontaneous polarization is calculated from the born effective charge of each atom in the different Wyckoff positions and the atomic displacements from equilibrium position of high symmetry phase. Figure 2(a) shows the spontaneous polarization in [001] ordered superlattice along the b-axis (P_s) which is closely related with moving CsI and RbI layers. In [001] ordered superlattice spontaneous polarization direction is related with moving of PbI layers.

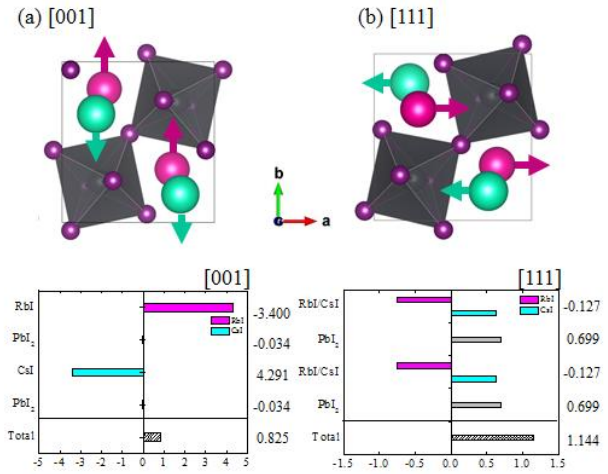

Figure 2. Berry phase polarization calculation from undistorted tetragonal phase to a fully distorted orthorhombic phase of (a) [001] projection of $CsRbPb_2I_6$ and (b) [111] projection of $CsRbPb_2I_6$.

The total polarization of [001] ordered superlattice is ~0.825 $\mu C/cm^2$ with approximately 93% of that value owing contributions from the CsI/RbI layers and the remainder from the two PbI_2 layers(Fig. 2a)..

Secondly we examined the spontaneous polarization for the [111] ordered superlattice (Fig. 2b). The total polarizarion of [111] superlattice is 1.114 $\mu C/cm^2$. Partial polarization calculations showed, that The total structural distortion for the PbI_2 compounds is larger than CsI and RbI compounds. The ferroelectric instability is larger for the PbI_2 compounds.

CONCLUSION

We have examined ferroelectric properties of $CsRbPb_2I_6$ superlattices. Spontaneous polarization was commonly found in [001] and [111] directions. The observed spontaneous polarization is expected to be one of the important properties which determines efficiency of perovskite based solar cells.

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