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# ANM Abstracts

Abstracts in session ANM for Plenary, Invited, Oral and Poster presentations

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# Electronic structure of $CsPbI_3/RbPbI_3$ cation ordered superlattices

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**ANM-nanomaterial-Poster**

## INTRODUCTION

Halide perovskites have recently emerged as promising materials for low-cost, high-efficiency solar cells[1]. Many studies have followed with the aim of both improving the performance of these materials in photovoltaic cells and of understanding which physical parameters may determine the efficiencies[2]. Good understanding of the structural and electronic properties is very important to predict new related functional materials.

## THEORETICAL STUDY

We have performed first principles density functional calculations of $CsRbPb_2I_6$ halyde perovskites with two different methods. The first approach is density functional calculations with the PBE-GGA approximation implemented in VASP [3]. The momentum space integrations were performed using a 5 × 4 × 4 Γ-centered Monkhorst-Pack *k*-mesh [4]. For the various symmetries examined, the lattice constants and internal coordinates were fully optimized until the residual Hellmann-Feyman forces became smaller than $10^{-6}$ eV/Å. Secondly, we have applied the hybrid density functional calculation of CRYSTAL09 [4] to study the electronic structure, especially to get the band gap energy.

## RESULTS AND DISCUSSION

Group theory analysis shows that $a^-a^-c^+$ octahedral tilting stabilizes the $Pmc2_1$ orthorhombic phase in the superlattice shown in Fig. 1(a). The large pink sphere represents a Cs ion and the small green sphere represents a Rb ions. $PbI_6$ octahedrals linked in *c* axis and have significant distortion and tilting. the The unit cell contains four formula unit for perovskite (20 atoms), and $Pmc2_1$ space group is actually a polar space group.

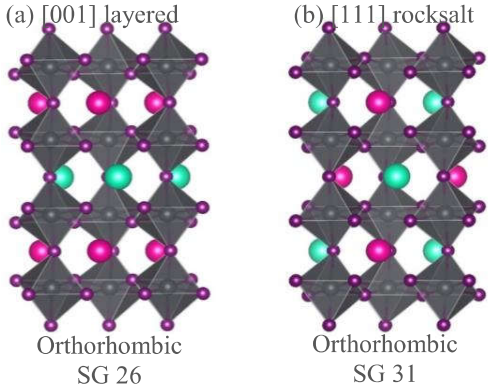


Figure 1. Structure of $CsRbPb_2I_6$ superlattices in [001] and [111] directions

We show in table 1. structural and electreonic properties of parent structures $RbPbI_3$, $CsPbI_3$ and superlattices in [100], [110], [111] directions within PBE and PBE0 approximation. In [100] direction the band gap value is 1.892 Ev and 2.68 eV respectively. In [110] direction the band gap value is 1.871 Ev and 2.70 eV respectively. Electronic structure of superlattices in [111] direction shows band gap value is 1.885 Ev and 2.63 eV respectively.

| Structure | Volume (Å$^3$) | Total E (eV) | $E_g$ PBE (eV) | $E_g$ PBE0 (eV) |
|---|---|---|---|---|
| $RbPbI_3$ | 478.83 | -28.202 | 1.922 | 2.86 |
| $CsPbI_3$ | 503.13 | -28.358 | 1.822 | 2.57 |
| $CsRbPb_2I_6$ [001] | 490.86 | -28.271 | 1.892 | 2.68 |
| $CsRbPb_2I_6$ [110] | 491.46 | -28.266 | 1.871 | 2.70 |
| $CsRbPb_2I_6$ [111] | 491.28 | -28.269 | 1.885 | 2.63 |

Table. 1 Structural and electronic properties of $RbPbI_3$, $CsRbI_3$ and $CsRbPb_2I_6$.

## CONCLUSION

We have examined the structural and electronic properties of ferroelectric compound $CsRbPb_2I_6$. We find the ground states of structures of the [100] and [111] ordered superlattices are polar. In all three directions the band gap value of PBE is underestimates ~70 % compared to that PBE0 hybrid functional calculation.

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