A Comprehensive DFT study of the structural and optoelectronic properties of orthorhombic perovskites $CH_3NH_3PbX_3$ (X = Br and I)

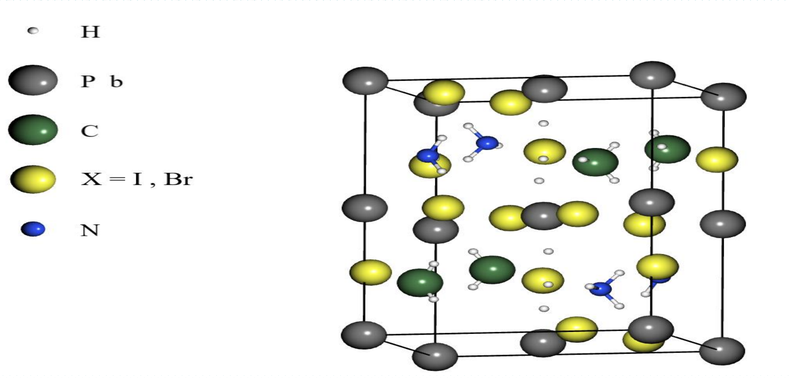
Soufiane Elhadfi[1]

1: Laboratoire d'Etude des Matériaux Avancés et Applications, Université My Ismail, Faculté des Sciences Meknes, Maroc

Abstract: The present study investigates the electronic and structural properties of the orthorhombic phase of the halogenated metal perovskite $CH_3NH_3PbX_3$ (X = Br and I), using density functional theory (**DFT**) methods. Based on extensive computational analyses, we explore the unique characteristics of this orthorhombic perovskite, including its electronic, structural, and optical properties. Our research has provided invaluable information on the behavior of this material, and results crucial to progress in the field of materials science.

Material description:

For the orthorhombic structure $CH_3NH_3PbX_3$ (X = Br and I), the organic cations CH_3NH_3+ are located in the interstitial spaces between the inorganic halogenated lead lattice. Lead ions (**Pb**) occupy positions within the structure, surrounded by both halogenated ions (**Br** or **I**) and organic CH_3NH_3 + cations. Halogen ions occupy specific positions, forming coordination bonds with lead ions.



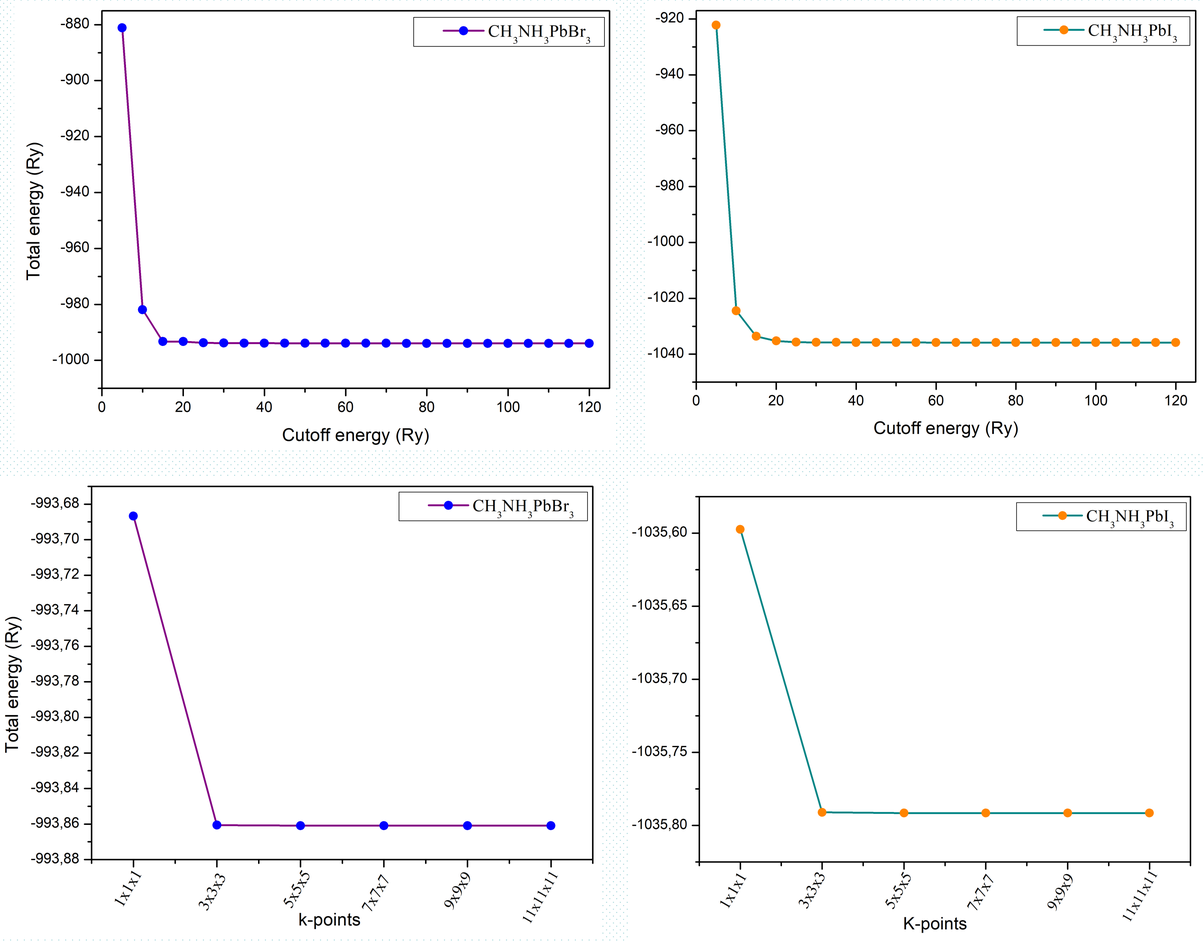
❖ Illustration of structure perovskites $CH_3NH_3PbX_3$ (X = Br and I)

Computational method:

The structural and electronic, are calculated using several types of methods. One of the most frequently used methods for determining the computational properties of compounds is the density functional theory, is the most accurate method for obtaining exploitable results. The structural and electronic properties of $CH_3NH_3PbX_3$ are investigated employing Quantum Espresso, this program calculates the Kohn-Sham eigenvalues within the framework of **DFT**, to optimize the structural systems, a 5×5×5 Monkhorst-Pack k-mesh was employed in the Brillouin zone, and the convergence threshold for the iteration of the SCF (self-consistent field) was set at 10^{-6} eV. Ions with the BFGS quasi-Newton algorithm have been relaxed to energies and forces below 1.0 Ry and 1.0 Ry/Bohr, respectively. The k mesh of 12×12×12 was used for the non-SCF and electronic calculations, with Gaussian smearing of 0.01 Ry. The cutoff values for the calculations convergence are 40 Ry for kinetic energy and 240 Ry for charge densities.

Results:

❑ Structural Properties:

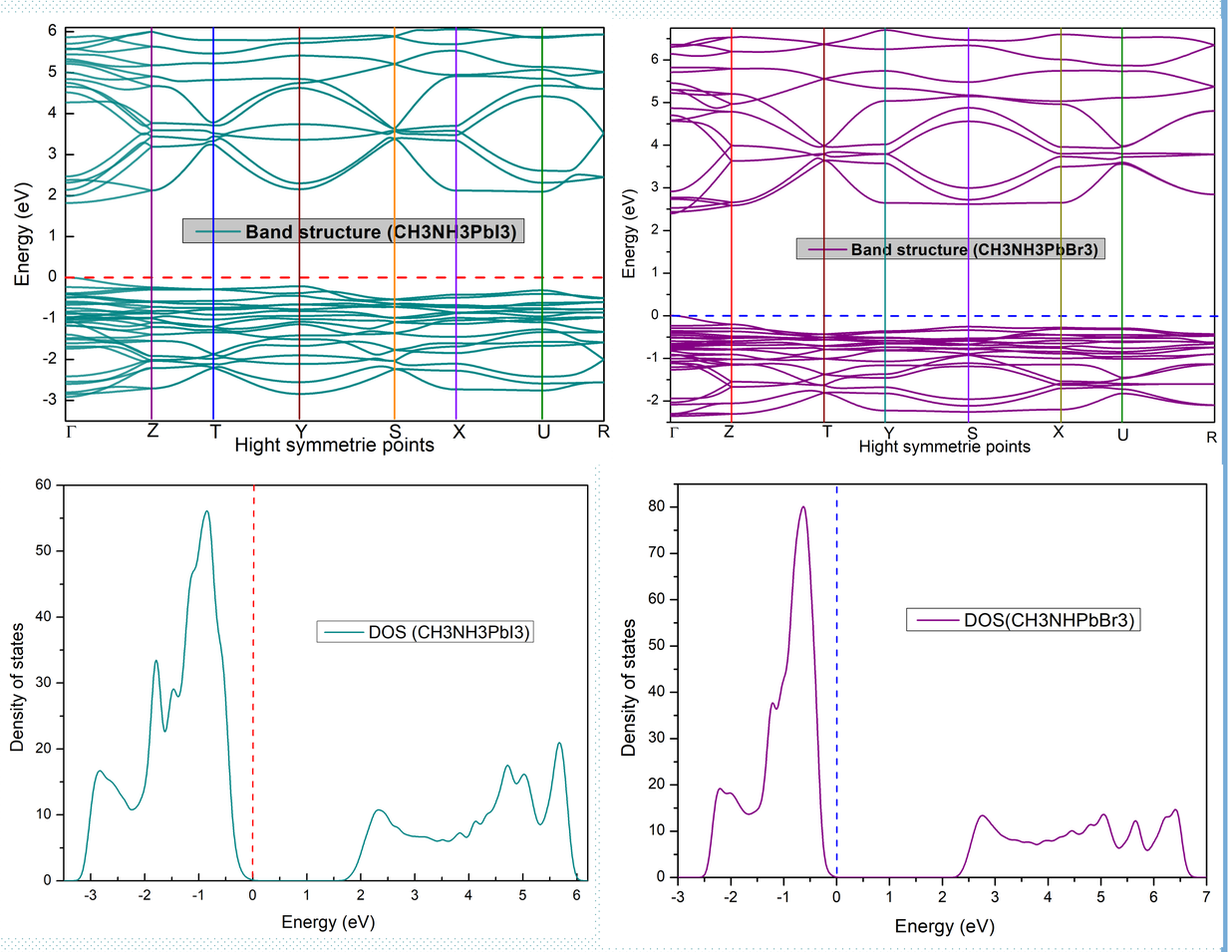


Cutoff and K-point Convergence for perovskites $CH_3NH_3PbX_3$ (X = Br and I)

❖ Table 1: The optimized lattice cell parameters compared with the experimental lattice.

$CH_3NH_3PbX_3$	This work			Experiments work [1,2]		
	a (Å)	b(Å)	c (Å)	a (Å)	b (Å)	c (Å)
$CH_3NH_3PbI_3$	8.53	9.27	12.27	8.84	8.55	12.80
$CH_3NH_3PbBr_3$	7.99	8.86	12.11	7.94	8.67	12.01

❑ Elecronic Properties:



the band structures and density of states of $CH_3NH_3PbX_3$ (X = Br and I) an orthorhombic perovskite calculated using the PBE/GGA functional. Successful comparison between our results and theoretical values previously accomplished using the same function. Also, the results are incredibly comparable with the experimental results(see Table 2) , confirming the adaptability of this functional. They are also very close to the experimental results, which shows that the function we used is adaptable.

❖ Table 2 : The band gap values in eV for $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$

E_g(eV)	This work	Experiments [1,2]	Other work [3]
$CH_3NH_3PbI_3$	1.82	1.90	1.80
$CH_3NH_3PbBr_3$	2.32	2.31	2.29

Conclusion:

The focus of the present research is on the structural and electronic properties of the orthorhombic perovskite $CH_3NH_3PbX_3$ (X = Br and I) has enabled us to acquire considerable background to this work. We have calculated the lattice parameters for the orthorhombic structures as well as those obtained in both structures experimentally, using the density functional theory of the first principle (DFT), with the generalized gradient approximation GGA. An examination of the electronic properties confirms that $CH_3NH_3PbI_3$ and $CH_3NH_3PbBr_3$ are direct bandgap semiconductor materials.

Refernces:

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