Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information : Orthorhombic lead-free hybrid perovskite $CH_3NH_3SnI_3$ under strain: An ab-initio study

Amina Dendane,[†] Benali Rerbal,[*,†] Tarik Ouahrani,[*,‡,¶,§] Alejandro Molina-Sanchez,[‖] Alfonso Muñoz,[⊥] and Daniel Errandonea[*,#]

†*Laboratory of Materials Discovery, Unit of Research Materials and Renewable Energies, LEPM-URMER. Université de Tlemcen 13000 Algeria., Algeria;*

‡*Ecole supérieure en sciences appliquées, ESSA-Tlemcen, BB 165 RP Bel Horizon, Tlemcen 13000, Algeria.*

¶*Laboratoire de Physique Théorique, Université de Tlemcen, Algeria.*

§*Université de Lorraine, Laboratoire Lorrain de Chimie Moléculaire, CNRS, L2CM, F-57000 Metz, France*

‖*Institute of Materials Science (ICMUV), University of Valencia, Catedrático Beltrán 2, E-46980 Valencia, Spain*

⊥*Departamento de Física, MALTA-Consolider Team, Universidad de La Laguna, San Cristóbal de La Laguna, E38200 Tenerife, Spain*

#*Departamento de Física Aplicada - Instituto de Ciencia de Materiales, Matter at High Pressure (MALTA) Consolider Team, Universidad de Valencia, Edificio de Investigación, C/Dr. Moliner 50, Burjassot, 46100, Valencia, Spain*

E-mail: ben.rerbal@gmail.com; tarik.ouahrani@univ-tlemcen.dz; daniel.errandonea@uv.es

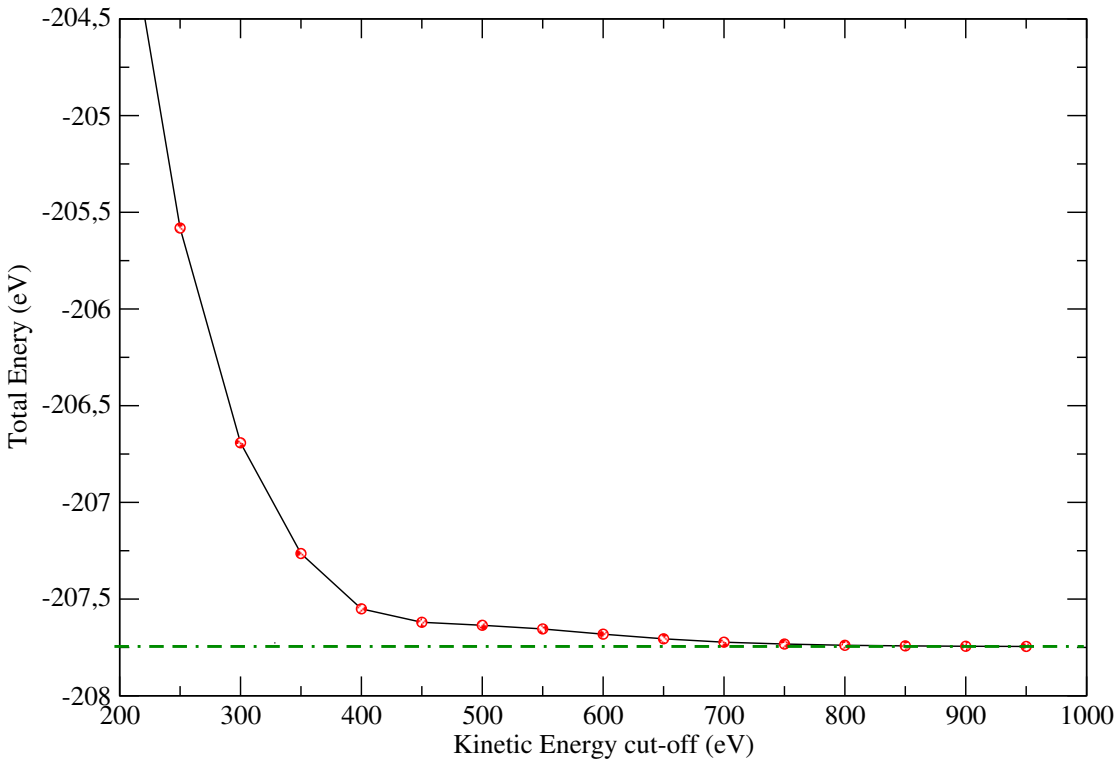

Figure S1 (Color online) The variation of the total energy as a function of the cutoff energy of un-strained $CH_3NH_3SnI_3$ hybrid perovskite

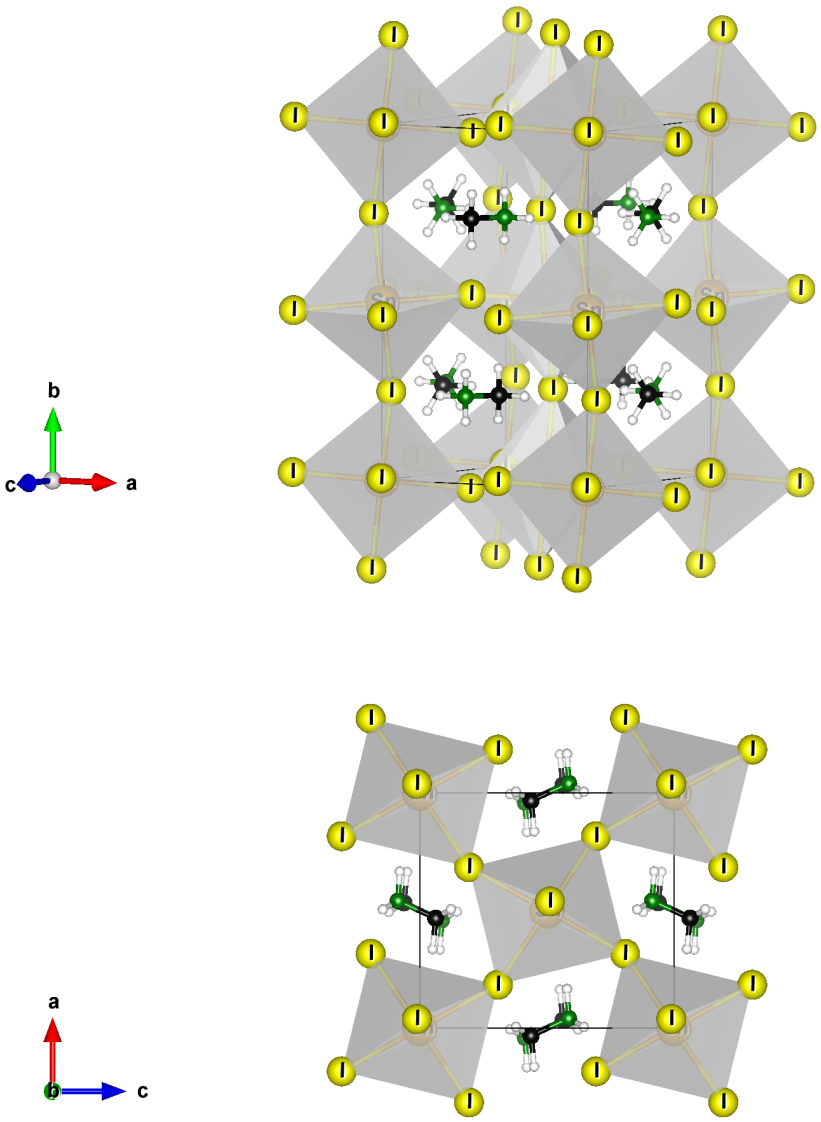

Figure S2 (Color online) Schematic view of orthorhombic $CH_3NH_3SnI_3$. The Sn, I, H, C, and N atoms are shown in orange, yellow, white, black, and green color, respectively.

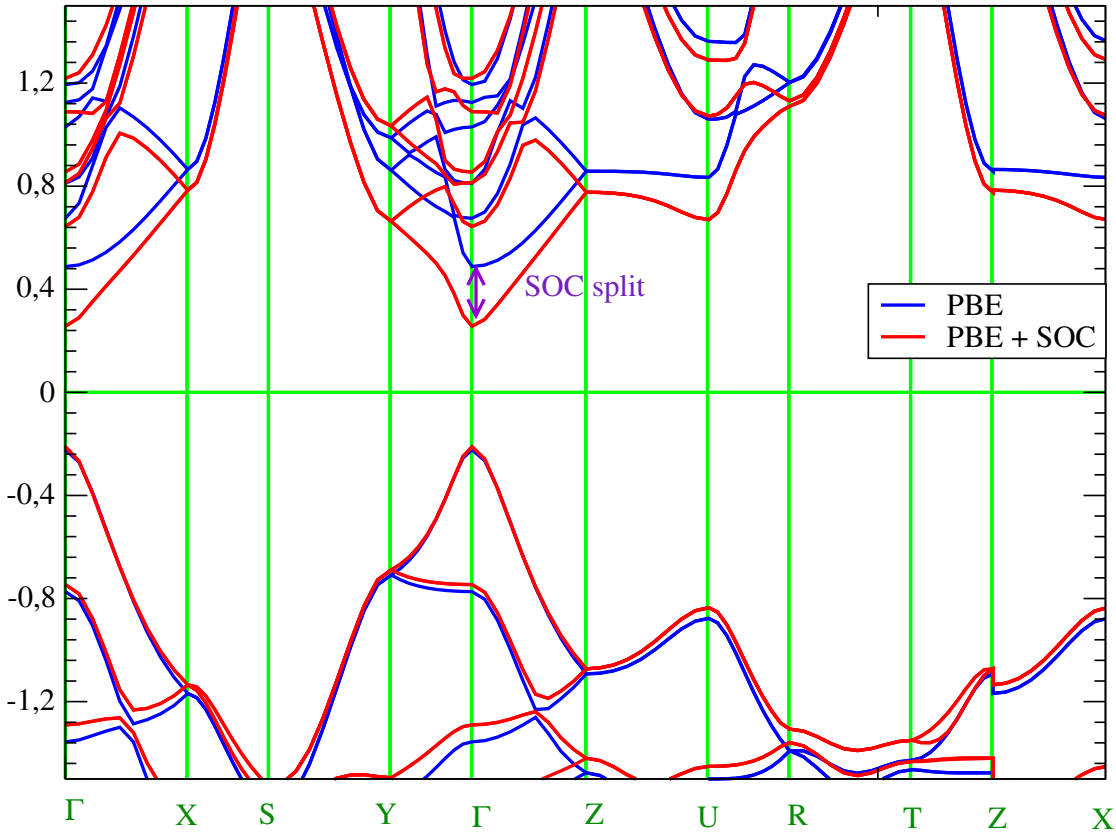

Figure S3 (Color online) Electronic band structure of $CH_3NH_3SnI_3$ calculated with spin-orbit coupling (SOC) (red line) and without SOC (blue line).