Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Stabilizing Tetramethylammonium Lead Iodide Perovskite and Exploring its Electronic and Optical Absorption for Solar cell Absorber Application

Ridwan O. Agbaoye

*Donostia International Physics Centre, Donostia San-Sebastian, Spain**

Paul O. Adebambo

Department of Physics, Federal University of Agriculture, Alabata Road, Abeokuta, Nigeria

Stephane Kenmoe

Department of Theoretical Chemistry, University of Duisburg-Essen, Universitatstr.2, D-45141 Essen, Germany

Gboyega A. Adebayo

Department of Physics, Federal University of Agriculture, Alabata Road, PMB 2240, Abeokuta, Nigeria†

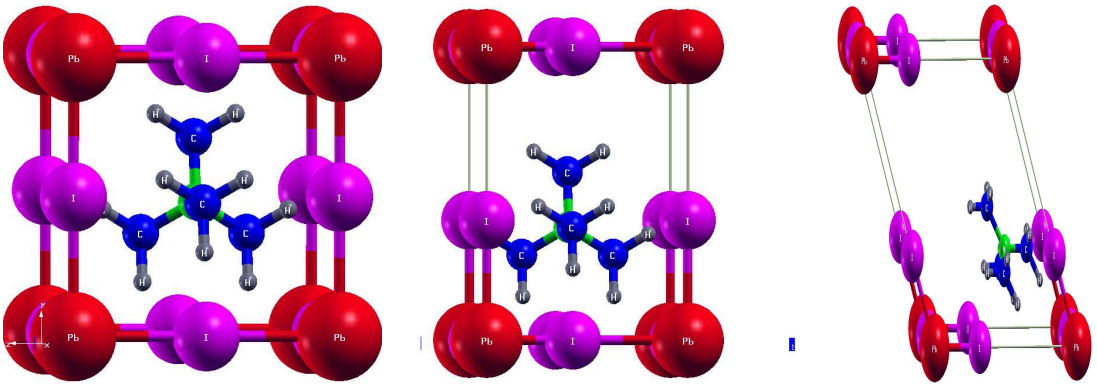

FIG. 1. (a) Cubic crystal structure of $(CH_3)_4NPbI_3$ (b) Tetragonal crystal structure of $(CH_3)_4NPbI_3$ (c) Hexagonal structure of $(CH_3)_4NPbI_3$

TABLE I. Lattice Parameters of Pseudo-Cubic, Tetragonal, and Hexagonal structured $(CH_3)_4NPbI_3$

	a ($\AA$)	b ($\AA$)	c ($\AA$)
This study (Pseudo-cubic)	6.35	6.44	6.34
This study (Tetragonal)	7.86	7.86	5.62
This study (Hexagonal)	9.77	9.77	7.91
Liu et al.,[1] (exp)	9.80	9.80	7.95
Jafarzadeh et al.,[2] (exp)	9.77	9.77	7.91

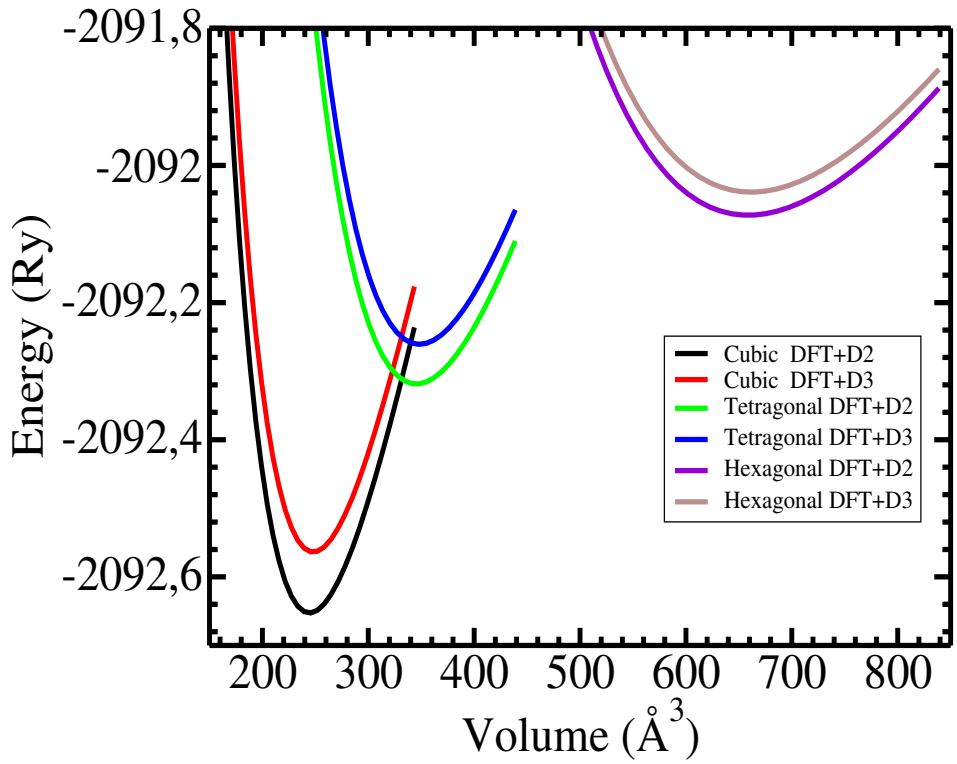

FIG. 2. Energy minimization of cubic, tetragonal and hexagonal structure of $(CH_3)_4NPbI_3$

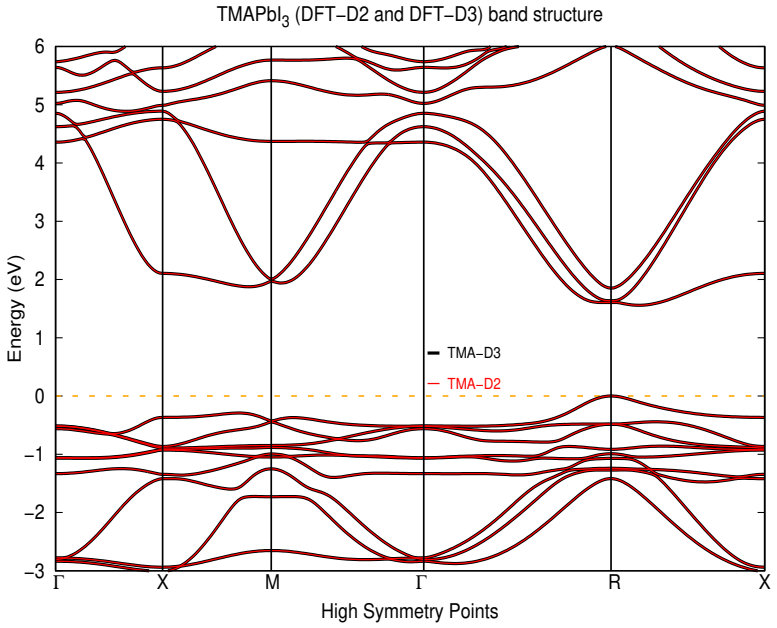

FIG. 3. DFT-D2 and DFT-D3 Electronic band structure of $(CH_3)_4NPbI_3$

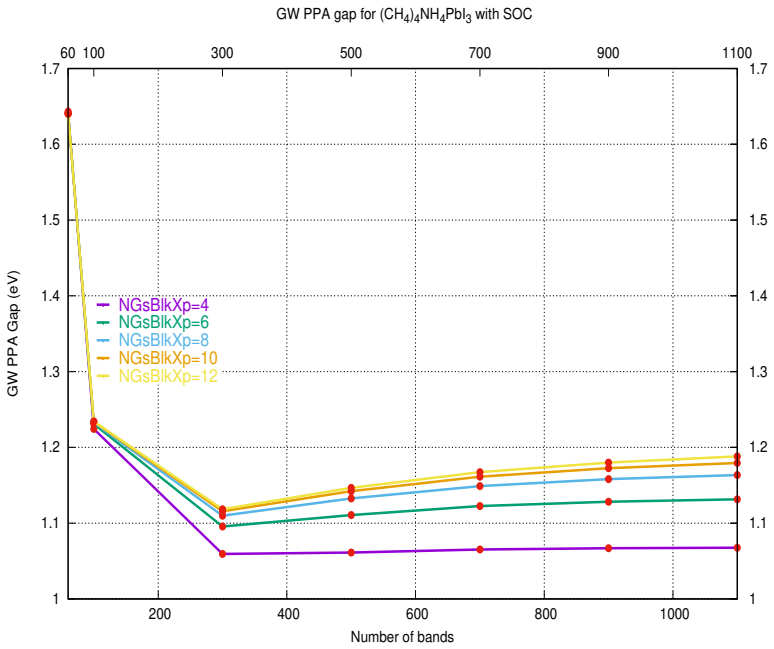

FIG. 4. GW PPA bandgap convergence with the number of bands for $(CH_3)_4NPbI_3$

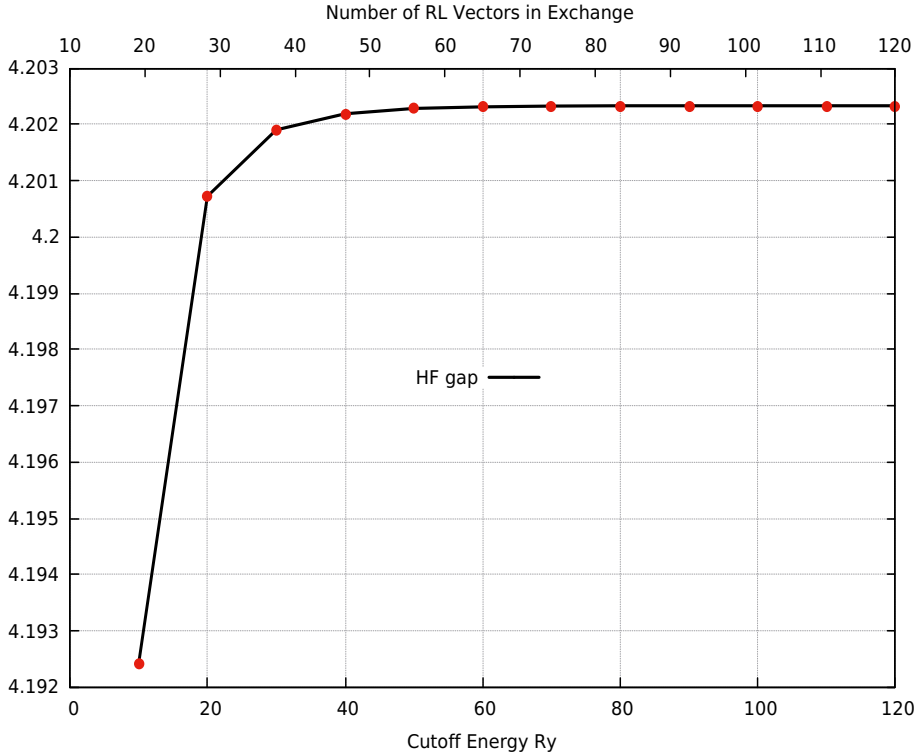

FIG. 5. The Convergence of the Number of Gvector in the exchange term with the Hartree Fock bandgap of $(CH_3)_4NPbI_3$ with spin-orbit coupling

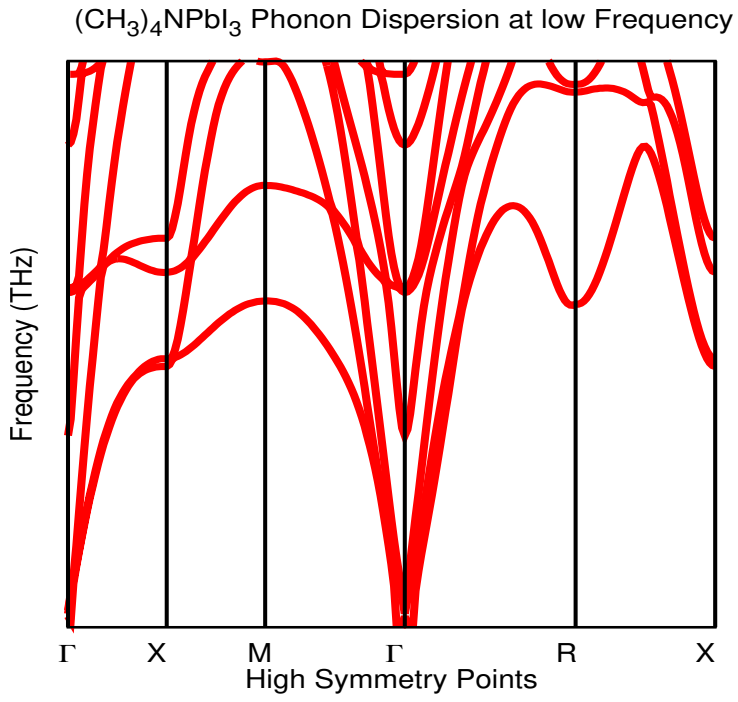

FIG. 6. Phonon dispersion of $(CH_3)_4NPbI_3$ at low frequency

TABLE II. DFT and DFT+soc and self-consistent GW band gap of $(CH_3)_4NPbI_3$

	With-SOC	Without-SOC
DFT (eV)	0.64	1.61
G_0W_0 (eV)	1.19	2.50
G_1W_1 (eV)	1.39	2.78
G_1W_0 (eV)	1.24	2.60
G_2W_2 (eV)	1.47	2.86
G_2W_0 (eV)	1.25	2.62
G_3W_3 (eV)	1.49	2.89
G_3W_0 (eV)	1.25	2.63

* ridwanolamide.agbaoye@dipc.org

† adebayo@physics.unaab.edu.ng

[1] G. Liu, J. Liu, Z. Sun, Z. Zhang, L. Chang, J. Wang, X. Tao, Q. Zhang, Thermally Induced Reversible Double Phase Transitions in an Organic–Inorganic Hybrid Iodoplumbate C4H12NPbI3 with Symmetry Breaking, Inorg. chem. 55, 8025 (2016). https://doi.org/10.1021/acs.inorgchem.6b01143.

[2] F. Jafarzadeh, S. Javadpour, M.H Shariat, Fabrication and investigation of a new highly humidity stable nanocrystalline perovskite, tetramethylammonium lead triiodide to be used in solar cells, Ceramics International,43,11552 (2017). https://doi.org/10.1016/j.ceramint.2017.05.030

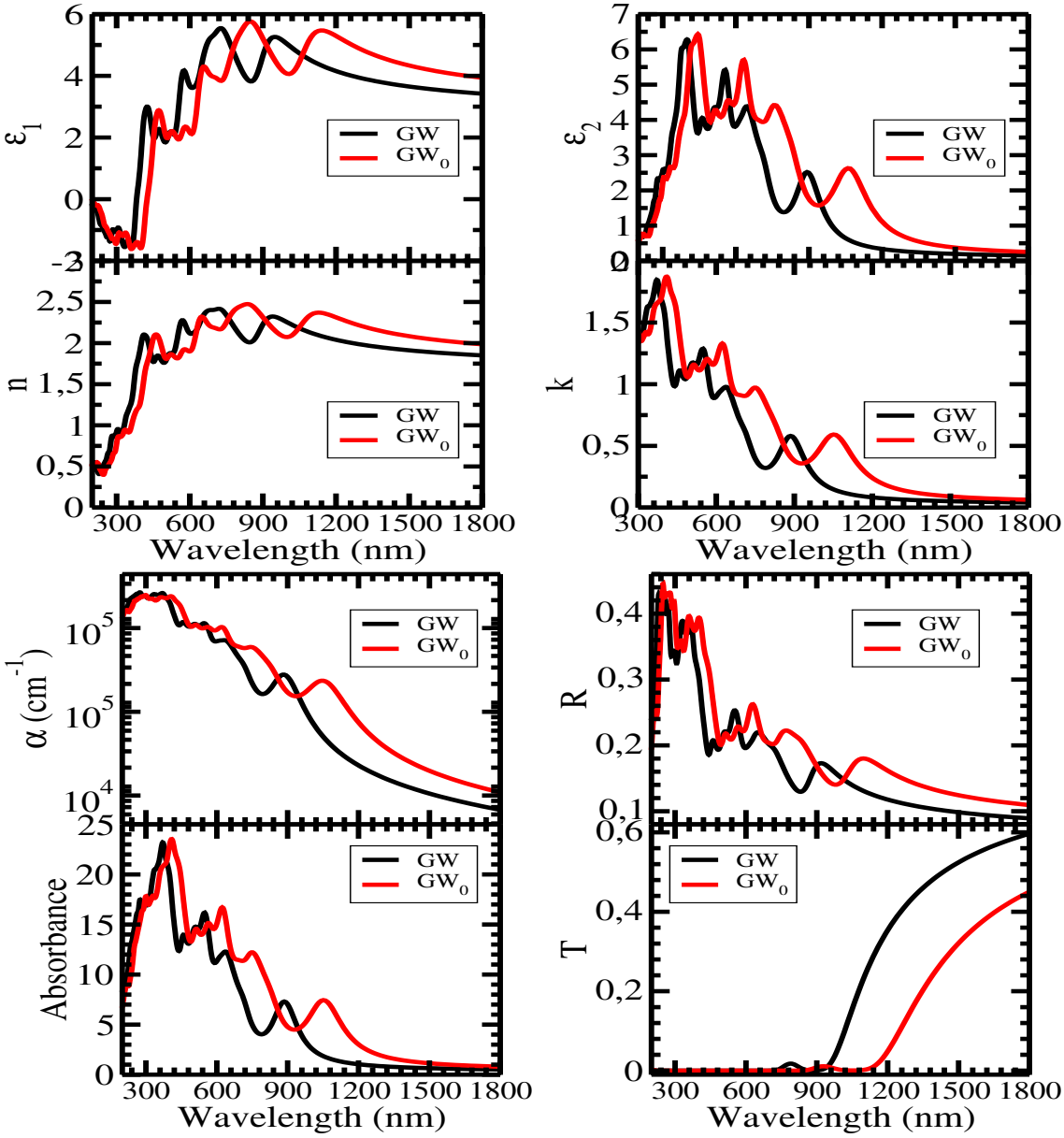

FIG. 7. BSE+SOC Optical spectra of $(CH_3)_4NPbI_3$(a) Real part of dielectric tensor (b) Imaginary part of dielectric tensor (c) Refractive index (n) (d) Extinction coefficient (k) (e) Reflectivity (f) Absorption coefficient (g) Absorbance (h) Transmittance