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REVIEWER'S REPORT

Manuscript No.: IJAR- 59790

Manuscript Title: Determination of the structural, electronic, and optical properties of the CH3NH3SiCl3 perovskite using an ab initio method.,

Recommendation:
Accept after minor revision

Rating	Excel.	Good	Fair	Poor
Originality		✔		
Techn. Quality			✔	
Clarity			✔	
Significance	✔			

Reviewer's ID: Bilqees Hamza

Detailed Reviewer's Repot

General Overview

The academic article titled "Determination of the structural, electronic, and optical properties of the $CH_{3}NH_{3}SiCl_{3}$ perovskite using an ab initio method" presents a first-principles Density Functional Theory (DFT) investigation of a lead-free hybrid organic–inorganic halide perovskite, methylammonium trichlorosilicate ($CH_{3}NH_{3}SiCl_{3}$), modeled in the cubic $Pm\text{-}3m$ phase. Using Quantum ESPRESSO with the PBE-GGA exchange-correlation functional ($E_{\text{cutoff}} = 80\text{ Ry}$, $10\times10\times10$ Monkhorst–Pack k-point mesh), the authors compute the equilibrium lattice constant ($5.72\text{ \AA}$), electronic band structure (yielding a direct bandgap of 2.509 eV at the R point), total and partial densities of states (TDOS/PDOS), and frequency-dependent optical spectra—including the complex dielectric function $\tilde{\epsilon}(\omega)$, refractive index $n(\omega)$, extinction coefficient $k(\omega)$, reflectivity $R(\omega)$, absorption coefficient $\alpha(\omega)$, optical conductivity $\sigma(\omega)$, and electron energy loss function $L(\omega)$.

A clear motivation of the manuscript is its focus on lead-free alternatives to toxic lead-based perovskites ($CH_{3}NH_{3}PbI_{3}$ and $CH_{3}NH_{3}PbCl_{3}$), offering a comprehensive set of electronic and optical response plots across the $0\text{--}20\text{ eV}$ energy spectrum to evaluate potential optoelectronic and UV-detector applications.

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However, to meet the standards required for academic publication, the manuscript requires major revisions to correct severe figure/data mismatches, copy-paste errors from unrelated compounds, erroneous equations, and internal numerical contradictions:

- **Wrong Compound Data and Copy-Paste Errors in Figures and Text:** Figure 3 (page 5), captioned *"Convergence of Kinetic energy cut-off ecut of $CH_{3}NH_{3}SiCl_{3}$ perovskite"*, actually displays a plot titled **"$NaSiAt_{3}$"** (sodium astatosilicate) rather than $CH_{3}NH_{3}SiCl_{3}$. Similarly, Figure 2 (page 3), captioned *"Convergence of Lattice Parameter of CH3NH3SiCl3 perovskite"*, plots **"PDOS (Etats/eV) vs. Energy (eV)"** on the axes instead of Total Energy vs. Lattice Parameter. In Section 3.3.1 (page 9, line 223), the text lists dielectric peaks *"for LiSiI3, NaSiI3, KSiI3, RbSiI3 and CsSiI3 respectively"*—inorganic alkali-metal iodides completely unrelated to $CH_{3}NH_{3}SiCl_{3}$. Furthermore, lines 92–100 (pages 3–4) contain an untranslated French paragraph immediately duplicated in English in lines 101–109.
- **Mathematical Errors in Optical Equations and Physical Contradictions:** In Section 3.3.2 (page 9), Equations (17) and (18) for the absorption coefficient $\alpha(\omega)$ and optical conductivity $\sigma(\omega)$ are identical copies of Equation (14) for the refractive index $n(\omega)$, while Equation (19) introduces an undefined symbol $I(\omega)$ without the required $1/c$ prefactor, and Equation (20) writes $\epsilon_{r}(\omega)$ in the numerator of $L(\omega) = \text{Im}[-1/\tilde{\epsilon}(\omega)]$ instead of $\epsilon_{i}(\omega)$. Additionally, Equation (13) contains a typo ($\epsilon_{r}(\omega') - 8$ instead of $\epsilon_{r}(\omega') - 1$). Physically, on page 8 (lines 184–186), the authors claim two electronic states lie *"entirely within"* the forbidden band gap—which is an artifact of Gaussian smearing in the PDOS plot rather than true mid-gap states—and on page 12 (lines 304–305), the text claims a non-zero *"static conductivity $\sigma(0)$ is $3.06 \times 10^{5}\text{ cm}^{-1}$"* for a semiconductor with a 2.509 eV band gap (and uses incorrect units for optical conductivity).
- **Internal Numerical Contradictions and Citation/Numbering Errors:** Across the Résumé (page 1), Section 3.3.2 (page 13), and Conclusion (page 14), the energy loss peak $L(\omega)$ is inconsistently reported as *"16.41–10.521 eV"* (confusing the y-axis peak height ≈ 16.41 with the x-axis energy position $\approx 10.52\text{ eV}$), *"6.53 at 7.42 eV"* (inverted coordinates of the smaller peak at $\sim 6.5\text{ eV}$ with height ~ 7.4), and *"maximum peak at 7.421 eV"* in the Conclusion. In the text on page 2 (line 58), Reference [22] is cited as *"Caputo, M. et al. focused instead on CH3NH3PbCl3 [22]"*, whereas [22] in the bibliography is

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the Quantum ESPRESSO paper by Giannozzi et al. (2009), and Caputo et al. is entirely missing from the References. Finally, figure numbering is broken throughout (two different figures are labeled "Figure 4", two are labeled "Figure 5", Figures 6–8 and 10 and 15 are skipped entirely), and duplicated raw OCR text appears beneath every figure.

Correcting the mislabeled plots ($NaSiAt_{3}$ and PDOS axes), removing unrelated compound references, fixing the optical formulas and EELS peak coordinates, and cleaning up the figure numbering and citations will be essential before the work can be considered for publication.