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Structural properties and stability study of Methoxybenzylamine-based Ruddlesden-Popper Lead Iodide Perovskite

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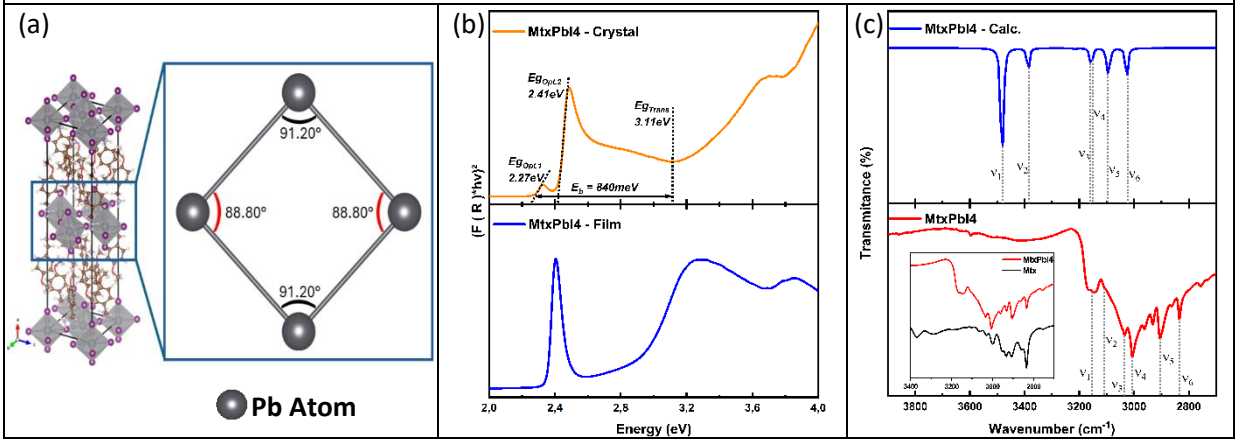
In recent years, the study of semiconductors has increasingly focused on perovskite compounds, owing to their promising optoelectronic properties. In this study, we investigated the stability of Mtx_2PbI_4 (where Mtx = methoxybenzylamine), a 2D Ruddlesden-Popper lead iodide perovskite, using various analytical techniques. The compound was characterized using single crystal X-ray diffraction (SCXRD). The SCXRD analysis (Fig. 1.a) revealed that Mtx_2PbI_4 crystallized in the orthorhombic space group Pbca (a = 34.11730; b = 8.83820; c = 8.65460; α = 90°; β = 90°; γ = 90°). Detailed analysis of the SCXRD data provided distortion parameters within the octahedral network (<D> = 3.1898 Å; ζ = 0.101154 Å; Δ = 0.000033; Σ = 24.3544°; Θ = 67.9116°; Vol = 43.17 Å³). Diffuse spectroscopy (Fig. 1.b) analysis enabled the calculation of the transmission bandgap of Mtx_2PbI_4 (3.11 eV), as well as optical bandgaps corresponding to excitonic states (2.27 eV and 2.41 eV), along with an excitonic binding energy of 840 meV. Infrared vibrational analyses (Fig. 1.c) provide insights into the influence of hydrogen bonds between layers on the octahedral structure of a single crystal. Furthermore, the stability of thin films of Mtx_2PbI_4 in polar (isopropanol) and non-polar (toluene) solvents was evaluated using diffuse and specular reflectance spectroscopy, demonstrating superior stability in non-polar solvents.

Figure 1. (a) Unit cell, (b) Tauc plot and (c) FTIR of Ruddlesden-Popper Mtx_2PbI_4..



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