

**CATIONIC INTERCALATION IN MOLYBDENUM DISULFIDE FOR
APPLICATION IN PEROVSKITE SOLAR CELLS**

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Perovskite solar cells (PSCs) have demonstrated remarkable progress in recent years, achieving impressive efficiencies of up to 27%. However, despite these advances, significant barriers hinder their large-scale commercialization. One of the main challenges lies in interface defects between the perovskite active layer and the charge transport layers, which lead to efficiency losses and degradation over time. To overcome this obstacle, additional material layers have been developed to assist in charge transport and device stability. This work proposes the synthesis of the metallic (1T) phase of the two-dimensional polymorph of molybdenum disulfide (MoS₂) intercalated with propylamine, for application in PSCs, aiming to improve the efficiency and stability of the device. While the semiconducting (2H) phase of MoS₂ assists in exciton dissociation, the 1T phase offers superior charge mobility, optimizing the electron transport. The synthesis involves the intercalation of lithium cations into the interlayer space of MoS₂ to alter the unit cell geometry, followed by hydration to facilitate the exfoliation of the compound. To adapt the material for deposition onto the perovskite layer, a cation exchange is performed, replacing Li⁺ with protonated propylamine. This modification prevents metal ion infiltration into the perovskite, minimizing hysteresis and preserving the integrity of the active layer.

Furthermore, the exchange enables the dispersion of 1T-MoS₂ in isopropanol (IPA), which is compatible with the perovskite layer. Characterization techniques employed for the synthesized compound included: X-ray diffraction (XRD) to confirm structural changes; differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) to evaluate thermal stability and composition; and Raman spectroscopy to identify characteristic vibrational modes of the 1T phase, indicating the efficiency of ionic intercalation and enhanced compound stability. The morphology of the material was analyzed using scanning electron microscopy (SEM), which enabled the measurement of the thickness and width of the exfoliated nanostructure. Preliminary results confirm the feasibility of applying the material in photovoltaic devices.

References:

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Acknowledgments:

National Institute of Organic Electronics (INEO), São Paulo Research Foundation (FAPESP), National Council for Scientific and Technological Development (CNPq) and Federal University of Technology of Paraná (UTFPR).

Palavras-chave: perovskite solar cell; interface engineering; molybdenum disulfide.