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Abstract

Organic-inorganic halide perovskite solar cells (Pero-SCs) have emerged as promising candidates for next-generation renewable energy technologies due to their exceptional power conversion efficiency and low manufacturing costs. However, the long-term stability and efficiency of Pero-SCs are significantly influenced by the choice of hole transport materials (HTMs). To address these challenges, we have conducted a comprehensive first-principles study to investigate the structure-property relationships of a series of newly engineered multifunctional coplanar π -conjugated HTM derivatives. Synergistic effect of design elements such as conjugation modification, heteroatom substitution, and fluorination on the electronic properties, hole mobility, molecular packing, and stability of these HTMs was investigated. The aim was to identify novel HTM candidates that could potentially outperform conventional Spiro-OMeTAD materials in terms of physiochemical stability and charge mobility. From results, fluorinated HTM derivatives with naphthalene conjugation backbone having thiophene and thiazole side fused units exhibited favourable electronic properties, including low-lying HOMO energies, high hole mobility, and efficient charge transfer characteristics. Notably, the incorporation of fluorine atoms into the molecular structure was found to enhance hydrophobicity, improve energy level alignment through push-pull mechanism, and facilitate charge carrier mobility with improved electronic coupling. Furthermore, the molecular packing and supramolecular interactions of the HTMs played a crucial role in determining their overall performance. Ordered π - π stacking and fibril network morphologies were identified upon controlled fluorination as key factors contributing to robust hole transfer as well as high hydrophobicity. Overall, this study provides valuable insights into the design and optimization of novel HTMs for Pero-SCs. The identified HTM candidates offer promising avenues for developing high-performance and stable Pero-SC devices, paving the way for their widespread adoption in renewable energy applications.

Keywords: Perovskite Solar Cells, Hole Transport Materials, Heteroatom Substitution, Controlled Fluorination, Conjugation Modulation

AI TECHNIQUES FOR OPTIMIZING CROP INSURANCE RISK

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Abstract

For sustainable Agriculture and food security to be ensured, accurate crop monitoring and forecasting are important. Agricultural landscapes are particularly vulnerable to extreme weather events, like heat waves, protracted droughts, and floods, which are the effect of climate change occurring more frequently and extremely. Farmers rely on crop insurance as a vital financial safety net to protect against losses caused by unpredictable weather conditions or natural disasters. Conventional crop insurance plans mainly depend on manual evaluations and historical data, which frequently fails to provide reliable risk estimates. Data is gathered from weather stations, field sensors, IoT devices, and earth observation satellites using Artificial Intelligence (AI) techniques. AI has the potential to improve risk assessment accuracy by utilizing machine learning and deep learning models, and predictive analytics. These tools