Molecular Passivation of ZnO Interfaces Using Self-Assembled Monolayers to Improve Electron Transport in Organic Photovoltaics

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As climate change intensifies, millions of lives are also increasingly threatened by energy insecurity, meaning renewable energy has become critical. Organic photovoltaics (OPVs) or organic solar cells offer a promising addition to traditional silicon-based solar cells due to their flexibility, low cost, and potential for integration into everyday materials such as windows, clothing, and indoor devices. However, OPV efficiency remains limited by poor electron transport layers, specifically zinc oxide (ZnO). This project explored the use of self-assembled monolayers (SAMs), which are ordered molecular layers that spontaneously form on a surface, to improve charge mobility and surface properties at the ZnO interface. Three SAMs, octadecanethiol (ODT), octadecyltrimethoxysilane (OTMS), and dodecanethiol (DDT), were deposited on ZnO films using spin coating and analyzed through current-voltage (J-V) measurements. Electron mobility was extracted using the Mott–Gurney law and space-charge-limited current curves. Among all tested SAMs, OTMS exhibited the highest electron mobility. To confirm this result, contact angle measurements were conducted, verifying successful SAM attachment and increased hydrophobicity. The superior performance of OTMS is attributed to its long alkyl chain and silane head group, which enable strong covalent bonding with ZnO surface hydroxyl groups, leading to uniform monolayer coverage, minimized trap states, and improved energy level alignment with the active layer. Furthermore, this study demonstrates that molecular-level surface engineering via SAM modification can improve OPV performance.

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