Stabilization of High-Performing Non-Fullerene Acceptor-Based Organic Solar Cells Using Naturally Occurring Antioxidants

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Abstract

Organic solar cells (OSCs) offer numerous advantages, yet their limited operational stability remains a key barrier to commercialization. Among the primary causes of performance decline is oxidative degradation within the organic active layer. Factors such as the molecular structure of the active materials, donor-acceptor miscibility, interfacial interactions, and film morphology all play vital roles in determining the extent of this degradation. The combined influence of light, oxygen, moisture, elevated temperatures, and potential impurities creates a highly reactive environment that accelerates chemical breakdown and loss of device functionality.

This thesis explores both the underlying principles of OSC operation and the degradation mechanisms that compromise device longevity. A particular focus is placed on the potential of antioxidant-based stabilization strategies to counter oxidative stress. A range of antioxidant classes, including hydrogen donors, hydroperoxide decomposers, and radical scavengers, were systematically evaluated for their effectiveness in suppressing degradation. Retinoic acid and curcumin emerged as especially effective due to their reactive oxygen species (ROS) neutralization capabilities and their role in maintaining charge transport integrity. Devices incorporating these antioxidants exhibited slower declines in power conversion efficiency (PCE) under continuous light exposure.

A comprehensive study was conducted on the impact of curcumin on both efficiency and stability across several donor-acceptor systems, including PBDB-T:ITIC, PM6:ITIC-2F, and PM6:Y7. The results showed that curcumin enhances both the initial PCE and the overall stability of OSCs.

To investigate the degradation mechanisms, techniques such as UV-Vis spectroscopy, Atomic Force Microscopy (AFM), and Photoluminescence (PL) were employed. PL measurements using DPBF and hydroethidine as probes identified two dominant degradation pathways: one driven by singlet oxygen and the other by superoxide anions. The prevailing mechanism was found to depend on the specific donor-acceptor pair.

In the final part of this research, attention was given to the impact of molecular structure on OSC behavior. Synthetic work carried out at the University of Copenhagen led to the development, purification, and characterization of subphthalocyanine (SubPc)-based organic semiconductors. When combined with existing organic photovoltaic systems and optimized fabrication techniques, SubPcs contributed to improved efficiency and stability of the resulting devices.