

A multi-modal approach to understanding degradation of organic photovoltaic materials

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State-of-the-art organic photovoltaic (OPV) materials are comprised of complex, chemically diverse polymeric and molecular structures that form highly intricate solid-state interactions, collectively yielding exceptional tunability in performance and aesthetics. These properties are especially attractive for semi-transparent power-generating windows or shades in living environments, greenhouses, or other architectural integrations. However, before such a future is realized, a broader and deeper understanding of property stability must be acquired. Stability during operating and environmental conditions is critical, namely: material color steadfastness, optoelectronic performance retention, morphological rigidity, and chemical robustness.

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Until now, no single investigation encompasses all four distinct, yet interconnected, metrics. Presented here is multi-modal strategy that captures a dynamic and inter-connected evolution of each property during the course of an accelerated photobleaching experiment. We demonstrate this approach across relevant length scales (from molecular to visual macroscale) using x-ray photoelectron spectroscopies, grazing incidence x-ray scattering, microwave conductivity, and time-dependent photobleaching spectroscopies for two high performance semi-transparent OPV blends – PDPP4T:PC60BM and PDPP4T:IEICO-4F, with comparisons to the stabilities of the individual components. We present direct evidence that specific molecular acceptor (fullerene vs non-fullerene) designs and the resulting donor-acceptor interactions lead to distinctly different mechanistic routes that ultimately arrive at what is termed “OPV degradation.” We directly observe a chemical oxidation of the cyano endcaps of the IEICO-4F that coincides with a morphological change and large loss in photoconductivity while the fullerene acceptor containing blend demonstrates a significantly greater fraction of oxygen uptake but retains 50% of the photoconductivity. This experimental roadmap provides meaningful guidance for future high-throughput, multi-modal studies, benchmarking the sensitivity of the different analytical techniques for assessing stability in printable active layers, independent of complete device architectures.