

Computational Spectroscopy for Organic Photovoltaics: Photodegradation of the D18 Organic Polymer

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Abstract. Organic photovoltaics (OPVs) offer an attractive route toward lightweight, flexible, low-cost, and environmentally friendly solar cells, and their efficiencies have now progressed to the level where they are competitive with current market-dominant devices. [1] However, their poor operational stability remains the central limitation to more widespread use. A mechanistic understanding of photo-induced degradation requires identification of the underlying degradation pathway. Assessing a theoretically proposed degradation pathway therefore requires linking it to an experimentally observable probe. Ideally, such a probe should be both element- and site-specific, allowing one not only to confirm the presence of mechanism-related elements, but also to resolve the local chemical environment sufficiently to identify the specific degraded site. In this work, we consider the photodegradation mechanism proposed by Kim and co-workers [2] and investigate it here as a possible degradation pathway in the highly efficient copolymer donor D18 [1]---known to exhibit stability problems under sunlight illumination. Using D18 as a representative model system, we examine how the ring-opening structural change modifies the excited-state and spectroscopic properties of the polymer. The aim is to explore the consequences of this degradation pathway and assess site-sensitive spectroscopic probes for locating the degraded site. To this end, we analyse the predicted effects of ring opening on UV/Vis, Raman, X-ray absorption, and resonant inelastic X-ray scattering [3] (RIXS) spectra. Particular emphasis is placed on RIXS as a site-sensitive probe of the local valence electronic structure at the degradation site, with Raman spectroscopy considered as a complementary vibrational probe of the degradation motif. Our results support the use of RIXS, together with Raman spectroscopy, as promising spectroscopic techniques for identifying local photodegradation motifs in organic photovoltaic materials.

REFERENCES

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