Dissipative engineering of environments for optimized photo-oxidation suppression in organic chromophores

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**Abstract:**

This work addresses the critical challenge of dye molecule oxidation and its impact on device stability by investigating the suppression of photobleaching through engineering the chromophore's surrounding environment. We induce strong coupling with confined light modes [optical cavities or localized surface plasmons (LSPs)] to reduce the triplet state population, thereby mitigating photo-oxidation. Utilizing the hierarchical-equations-of-motion (HEOM) approach to capture non-Markovian and non-perturbative effects, we analyze both cavity-chromophore and LSP-chromophore systems. Our analysis reveals that the optimal antioxidation performance depends on the competition between cavity-chromophore coupling and cavity-bath (dissipation) interaction. Importantly, in the strong cavity-chromophore coupling regime, increasing cavity dissipation can enhance antioxidation through quantum coherence-induced population transfer. Conversely, in the weak cavity-chromophore coupling regime, increasing cavity dissipation can counterintuitively reduce the antioxidation capability due to a quantum Zeno-like effect. Furthermore, in the LSP-chromophore system, engineering the LSP structure, particularly the LSP dissipation rate, can similarly be used to optimize the antioxidation effect. These findings, complemented by analytical results for finding optimal system parameters, provide practical guidelines for designing photostable organic materials with enhanced performance in various optoelectronic applications.