**Chemical degradation of OLED host materials: the role of excited carriers in non-local interaction**

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Despite the conspicuous advances in organic light-emitting devices (OLEDs) and even their successful implementation in commercial displays, device degradation still remains as the most important issues. Because degradation occurs mostly in working conditions, the underlying mechanism is thought be linked to excited state of carriers. While several theoretical and experimental studies have focused on the mechanisms of OLED degradation, the microscopic role of the excited carrier remains elusive. In this work, using occupation-constrained density functional theory calculations, we study how chemical degradation is driven by the excited carrier in OLED host materials. We show that the C-N bond is a weak link of the OLED molecules both in the electronic ground and excited states, and the rupture of the bond is the main cause for chemical degradation. While the excited carrier generally weakens the bond, the effect can be mitigated by the non-local interaction with the other bonding and anti-bonding states. We suggest that the presence of such a non-local interaction can contribute to an enhancement of the chemical stability in the excited state.

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