

π -Topology, Ultrafast Excited-State Dynamics, and FET Performance of Remarkably Photochemically Stabilized Pentacene Derivatives with Radical Substituents

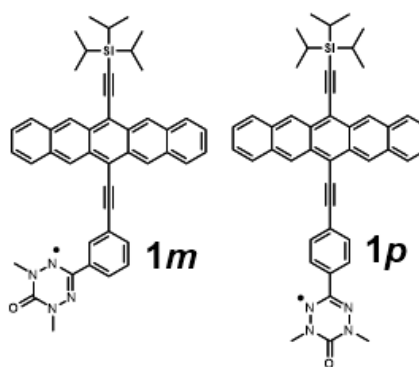
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In our previous works, we reported a novel strategy for the photochemical stabilization (radical photostabilization) that utilized the unique excited-state spin dynamics induced by the attachment of the π -radical substituent(s) to the pentacene (Pn) moiety [1-3]. Thus, Pn derivatives with one or two π -radical substituent(s) were significantly more stable against photodegradation because of the enhanced/accelerated intersystem crossing (EISC) of the Pn moiety. In the present work [4], we report novel pentacene-radical-linked systems (**1m** and **1p**) with the topologically different π -orbital networks (π -topology). They showed a remarkable improvement in photochemical stability, which was 187 (139) times higher than that of 6,13-bis(triisopropylsilyl)ethynyl)pentacene (TIPS-Pn). Transient absorption (TrA) spectroscopy showed that this remarkable photostabilization is due to the ultrafast intersystem crossing induced by effective π -conjugation between the radical substituent and pentacene moiety owing to their molecular planarity. It is also worthy of notice that the intersystem crossing of the purely organic compounds without heavy atoms is realized in the sub-femtosecond region. The relationship between π -topology and the photochemical stability is also discussed based on the excited-state dynamics. In addition, π -topological control of the excited-state dynamics was realized and applied to the enhancement of photochemical stability. Field-effect-transistor (FET) performance was also evaluated using **1m** and **1p** as the hole transport materials.



[1] Y. Kawanaka, A. Shimizu, T. Shinada, R. Tanaka, Y. Teki, *Angew. Chem. Int. Ed.* **52**, 6643 (2013). [2] A. Ito, A. Shimizu, N. Kishida, Y. Kawanaka, D. Kosumi, H. Hashimoto, Y. Teki, *Angew. Chem. Int. Ed.* **53**, 6715 (2014). [3] A. Shimizu, A. Ito, Y. Teki, *Chem. Commun.* **52**, 2889 (2016). [4] N. Minami, H. Hashimoto, Y. Teki et al., *Phys. Chem. Chem. Phys.* accepted [DOI: 10.1039/d2cp00683a] [back cover].