Synthesis and photophysical properties of pentacene triangular macrocycle

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Triangular-shaped molecules are a class of macrocycles that has been widely studied. Rigid triangular macrocycles composed of organic chromophores substituted with aliphatic chains can form controllable supramolecular networks. These networks can introduce novel functionalities for applications in optoelectronics and energy conversion. Singlet fission (SF) is a multi-exciton generation process that generates two individual triplet excitons ($T_1 + T_1$) from a correlated triplet exciton pair (TT) in two nearby molecules after one-photon absorption ($S_1 + S_0$). The long-lived triplet excitons can enable us to demonstrate efficient intermolecular exciton diffusion by molecular assembly in thin film. Pentacene is one of the typical candidates that satisfies the energy matching conditions for the occurrence of SF. In this work, pentacene units were newly introduced into a triangular macrocycle system with suitable aliphatic chains for supramolecular assemblies (Fig. 1).

Two pentacene moieties are successfully introduced through a series of reactions in combination with dialkoxy benzene linkers. These long alkyl chains were also introduced in the linkers and can easily be modified in the synthetic of the starting material.⁴ The supramolecular formations can be controlled for intermolecular exciton transport by carefully designing the chain lengths. Moreover, the triangular pentacene dimer Tri(Pc)₂ synthesis can be a prospective synthetic route for the synthesis of other shape-persistent pentacene derivatives that would potentially have inquisitively singlet fission properties.⁵

Figure 1. Synthetic strategy of triangular pentacene dimer

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