Amide-Embedded π-Conjugated System: Functional Exploration of Amide Bond as Polar Double Bond Alternative

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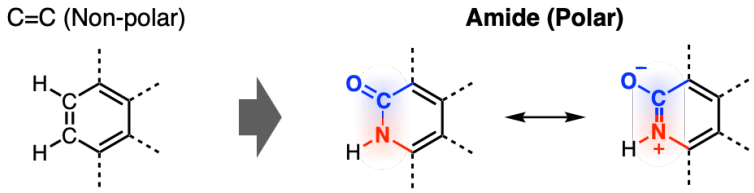
Polycyclic aromatic hydrocarbons (PAHs) with in-plane dipole moments are promising materials for optoelectronic materials.[1,2] This is because the in-plane dipole moment can lead to the separation of frontier molecular orbitals (FMOs) and enhanced intermolecular interactions. In this study, we have reported amide-embedded PAHs, where C=C bonds are substituted with amide bonds, which exhibit double bond character and large dipole moments due to the contribution of the resonance structure.[3] Spectroscopic analyses and DFT calculations reveal that embedded amides significantly change FMO distributions and achieve reduced band gaps, high triplet energies, and high fluorescence quantum yields. In addition, hydrogen bonding of embedded amide can control crystal structure, presenting a novel crystal engineering strategy for π-conjugated systems.[4]



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