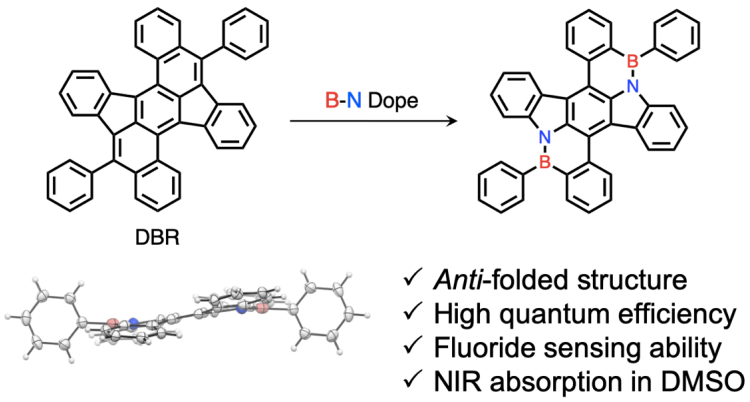
B_2N_2-Doped Dibenzorubicene; Synthesis and Properties

(School of Science, The University of Tokyo)
○Takumi, Sakamaki; Rui, Shang; Eiichi, Nakamura

Keywords: Isoelectronic analogues; Heteroaromatics

Abstract: Curved π-conjugated molecular have attracted much interest because they have good solubility and unique properties compared to planar π-conjugated system. On the other hands, doping boron-nitrogen (B-N) unit into π-conjugated system is effective strategy to tune optical and physical properties. Considering the isoelectronic relationship between C=C and B-N bonds, replacement of the C=C units in π-skeletons with the corresponding B-N units would create a new type of heteroarene that maintains the structural similarity. For example, BN doped π-conjugated system usually have high luminescence due to dipolar nature BN unit. With boron atom has Lewis acidic property because of vacant p-orbital.

In this work, We designed and synthesized a new BN-doped molecule based on these two strategies. The dibenzorubicene (DBR) backbone has nonplanar structure and high charge career mobility, which can be used for optoelectronic devices,[1] but it has low quantum efficiency. By doping BN unit properly located in a nonplanar molecule, the fluorescence quantum yields of compounds were up to 88%. In addition, high sensitivity of fluoride ion was achieved maintaining strong fluorescence, indicating the efficient emission properties of these materials. Achiral *anti*-folded backbone of BN compound was revealed by single-crystal X-ray structure analysis. Interestingly, When BN compound was dissolved in DMSO, near infrared (NIR) absorption could be observed. The application of these materials in various organic devices is expected.



1) X. Gu, X. Xu, H. Li, Q. Miao, *J. Am. Chem. Soc.* **2015**, *137*, 16203–16208.