Exciton-driven Bulk Photovoltaic Effect in Polar Organic Crystals with Subphthalocyanines

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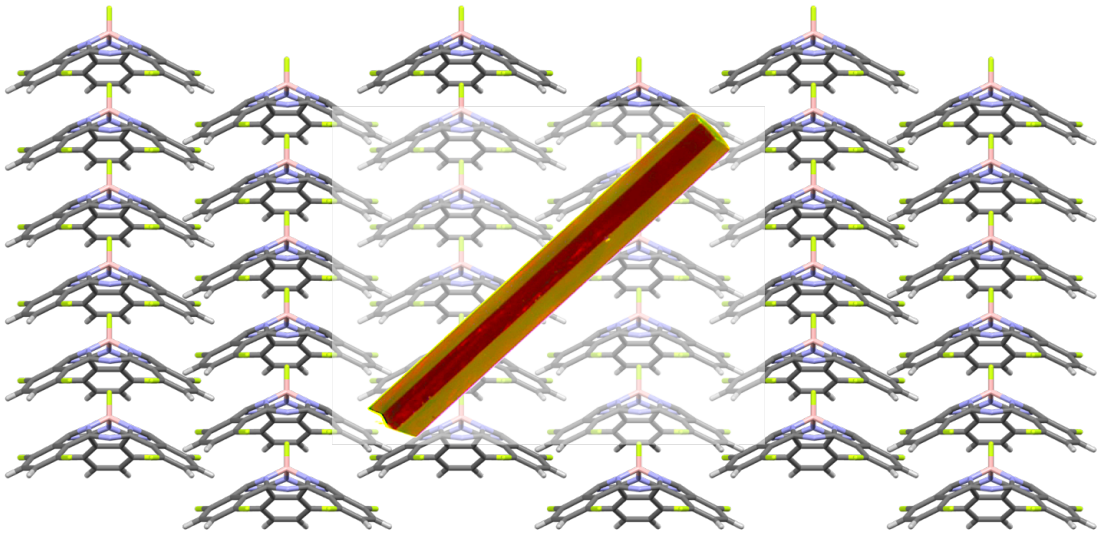
Keywords: Bulk Photovoltaic Effect; Exciton; Charge Transfer; Shift Current; Subphthalocyanine

Polar materials attract wide research interest due to their unique properties, such as ferroelectricity and the bulk photovoltaic effect (BPVE)[1)], which are not accessible with nonpolar materials. However, in general, rationally designing polar materials is difficult because nonpolar materials are more favorable in terms of dipole-dipole interactions. Recently, we reported a rational strategy to form polar assemblies with bowl-shaped π-conjugated molecules and a molecular design principle for this strategy[2)]. Based on this design principle, we successfully developed more than 12 polar crystals. Furthermore, we unveiled that the BPVE observed in these polar assemblies is generated in the shift current mechanism. This presentation will overview the design principle and discuss the relationship between excitation and photocurrent generation[3)].



1) C. Zhang *et al*., *J. Am. Chem. Soc.*, **2020**, *142*, 3326. 2) C. Zhang *et al*., *Angew. Chem. Int. Ed.*, **2021**, *60*, 3261. 3) B. Dhara, *et al*, *to be submitted*.