

## **Effect of graphene between photoanode and sensitizer on the intramolecular and intermolecular electron transfer process**

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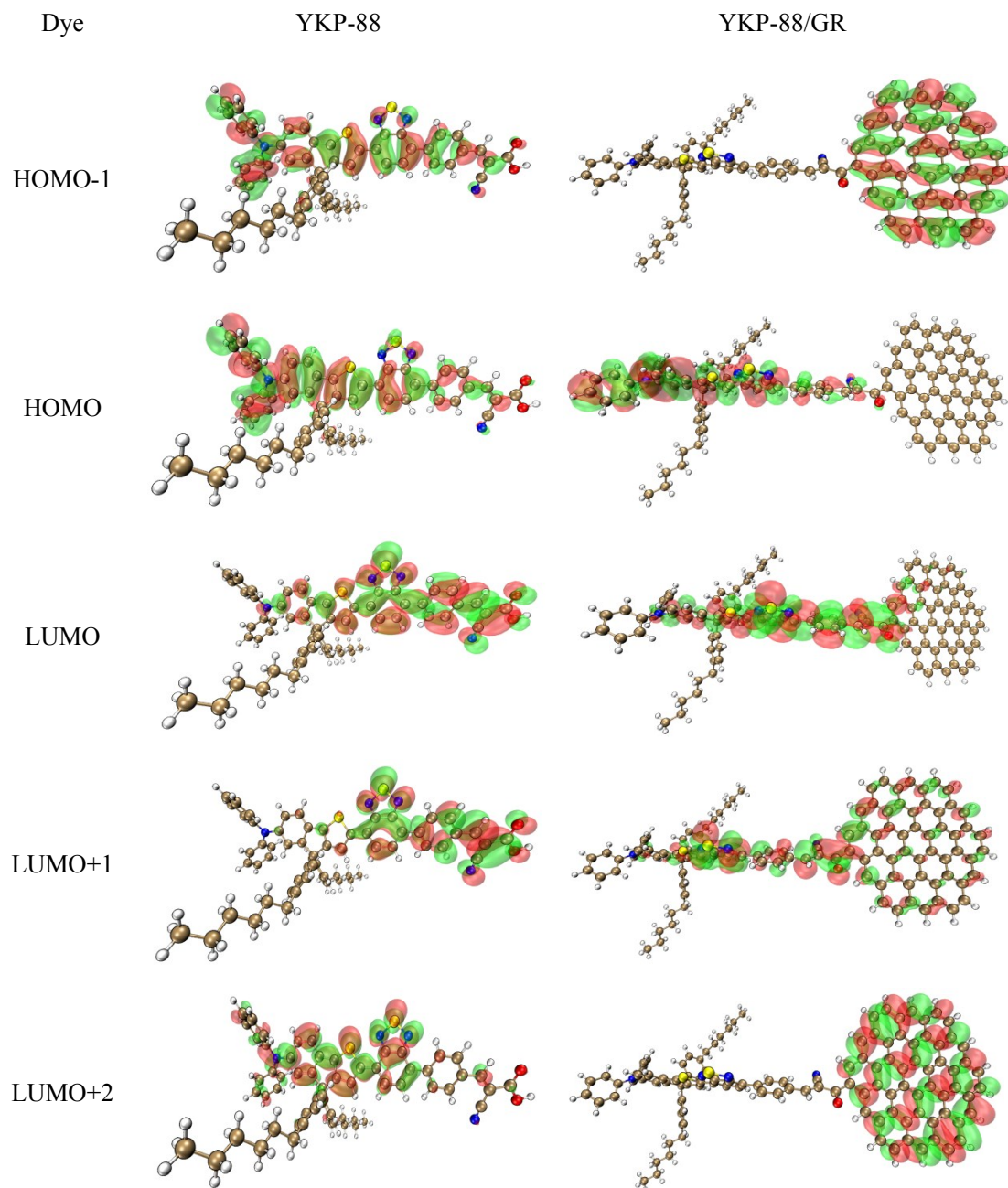
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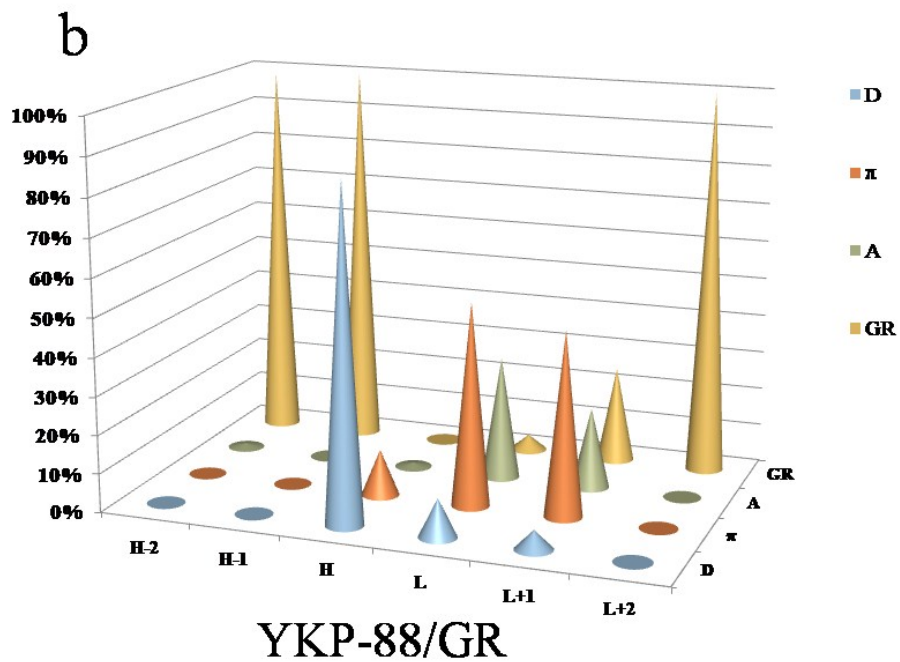
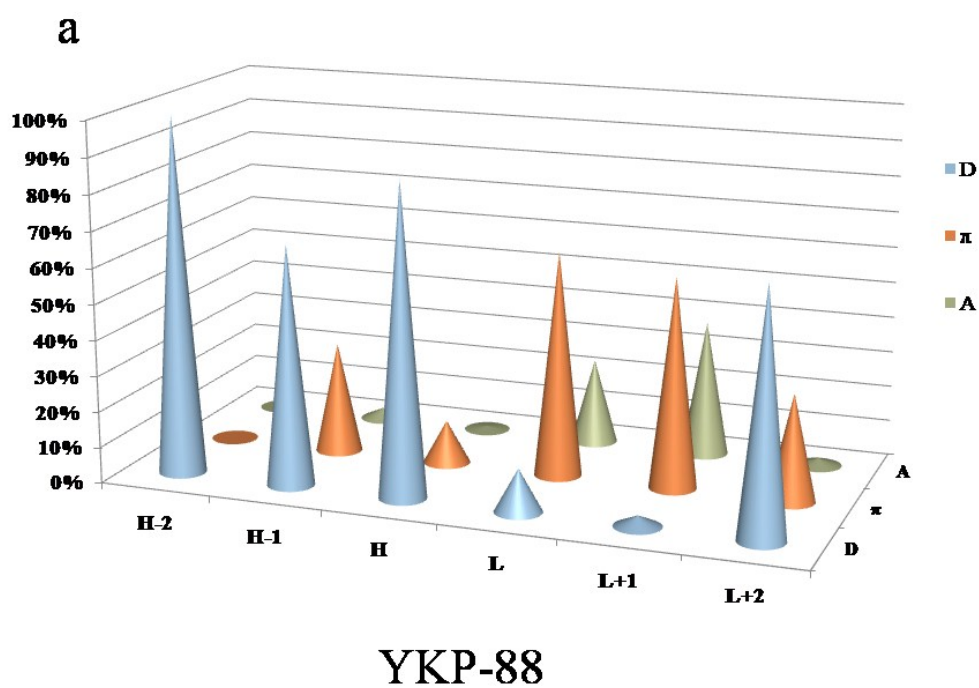
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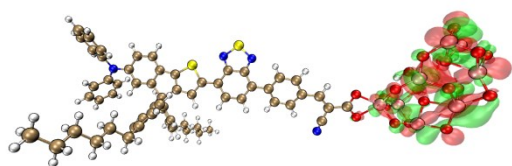


**Figure S1** Frontier molecular orbitals of YKP-88 and YKP-88/GR.

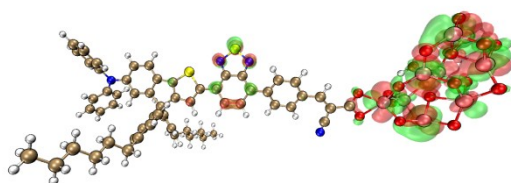


**Figure S2** Electron density proportion of the individual groups in occupied orbitals (HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1 and LUMO+2 ) of the dye and its graphene complexes (a represents dye; b represents its graphene complexes).

YKP-88@(TiO<sub>2</sub>)<sub>16</sub>

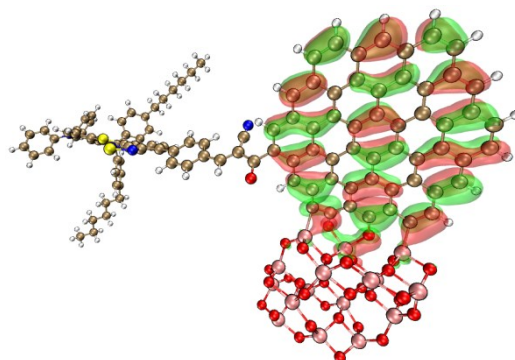


LUMO+5

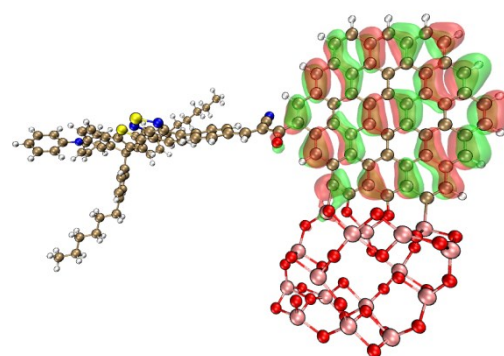


LUMO+7

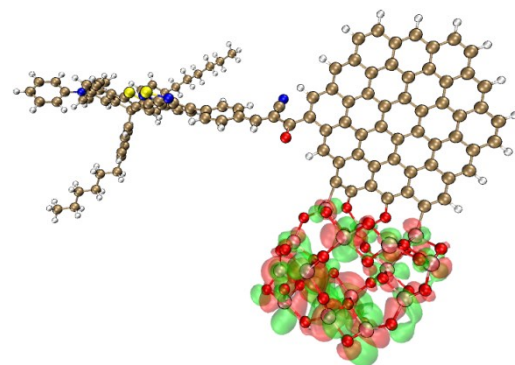
YKP-88/GR@(TiO<sub>2</sub>)<sub>16</sub>



HOMO-2

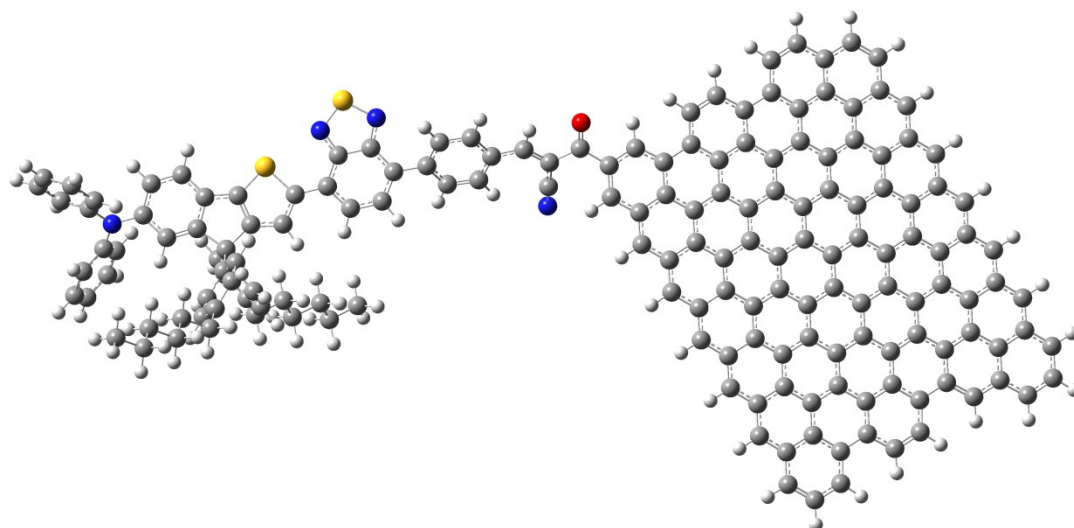


HOMO-1



LUMO+3

**Figure S3** Frontier molecular orbitals of YKP-88@(TiO<sub>2</sub>)<sub>16</sub> and YKP-88/GR@(TiO<sub>2</sub>)<sub>16</sub>.



**Figure S4** Geometrical structure of YKP-88@GR.