Supporting information for: Theoretical study of D-A'-π-A / D-π-A'-π-A triphenylamine and quinoline derivatives as sensitizer for dye-sensitized solar cells

Ying Zhang,^{‡a} Ji Cheng,^{‡a} Wang Deng,^{‡b} Bin Sun, ^c Zhixin Liu,^a Lei Yan, *^a Xueye Wang, *^aBaoming Xu,*^b Xingzhu Wang *^{a,b}

- ^a College of Chemistry, School of Physics and Optoelectronics, Xiangtan University, Xiangtan, Hunan Province 411105, China
- ^b Department of Materials Science & Engineering and Academy for Advanced Interdisciplinary Research, Southern University of Science and Technology, Shenzhen, Guangdong Province 518055, China,
- ^c North China Sea Marine Forecasting Center of Ministry of Natural Resources, Qingdao, Shandong Province 266000, China

*Corresponding authors.

E-mail addresses: xz_wang@hotmail.com (X.Z. Wang); yanlei@xtu.edu.cn (L. Yan);wxueye@xtu.edu.cn (X. Wang); xubm@sustech.edu.cn(B.Xu)

‡ Those authors contributed equally.

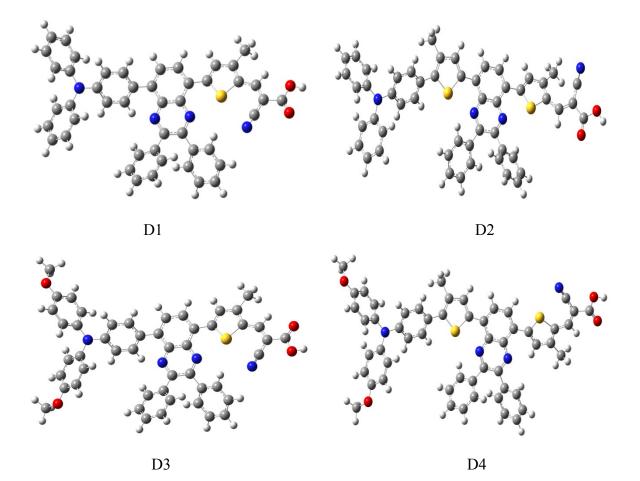


Figure S1. The optimized structures of dyes D1-D4 by DFT//B3LYP/6-311G(d,p)