

## Can fused-pyrrole rings act as better $\pi$ -Spacer units than fused-thiophene in dye-sensitized solar cells? A computational study

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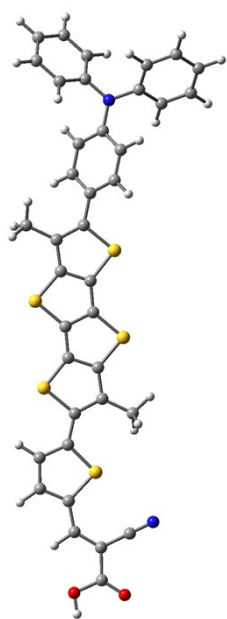
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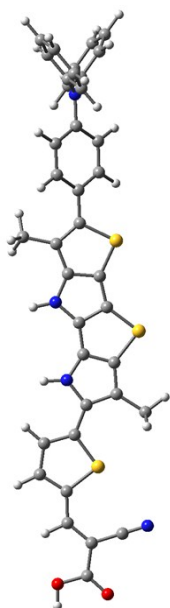
### Supporting Information:

**Table S1:** The calculated atomic charge distribution with NBO 3.1 (in e) of the  $(\text{TiO}_2)_{10}$  of **1-**  
 **$(\text{TiO}_2)_{10}$**  and **3-** **$(\text{TiO}_2)_{10}$**  and dipole moment ( $\mu_{\text{normal}}$ ).

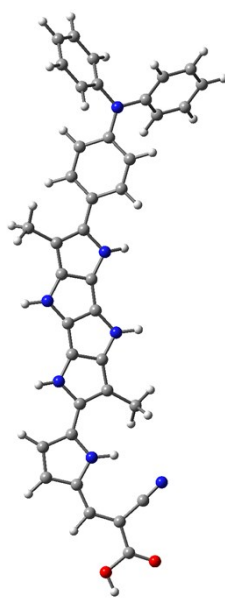
$S_0$		$S_1$		
Dyes	$(\text{TiO}_2)_{10}$	$\mu_{\text{normal}}$	$(\text{TiO}_2)_{10}$	$\Delta q$
<b>1</b>	0.373	8.54	0.256	0.117
<b>3</b>	0.307	12.94	-0.588	0.895



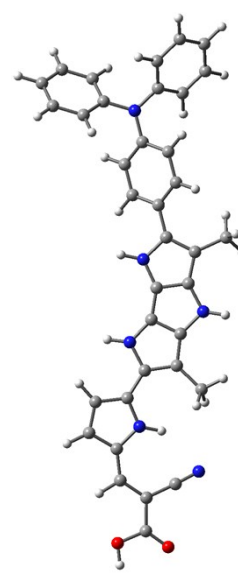
dye 1



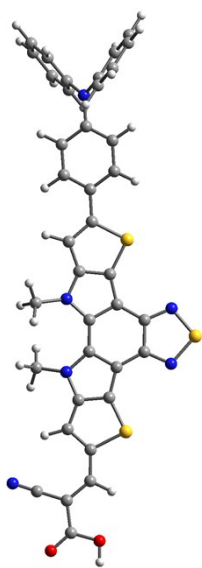
dye 2



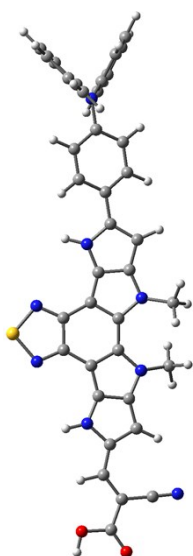
dye 3



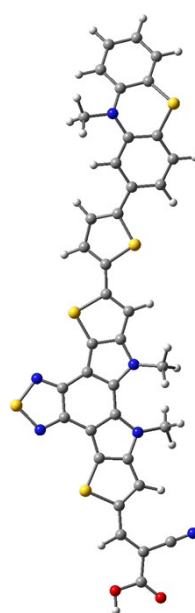
dye 4



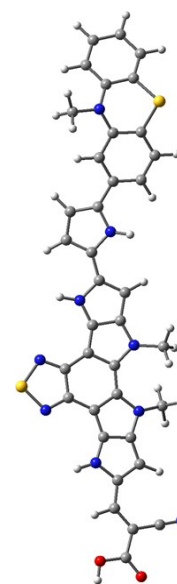
dye 5



dye 6



dye 7



dye 8

**Figure S2:** Most stable optimized structures of the dyes 1-8.