

## **Supplementary Information**

**Fullerene-based materials for solar cell applications: Design of novel acceptors for efficient polymer solar cells-a DFT study**

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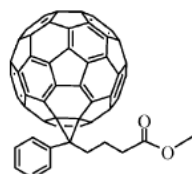
**Phone: +98-7136137161. FAX: +98-7136460788.**

**Table S1.** Basis set performance for PC<sub>60</sub>BM

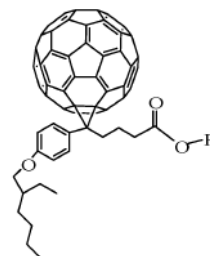
	Basis set	HOMO-LUMO gap(eV)	$\eta$ (eV)	$\gamma$ (eV)	$\alpha$ $\text{\AA}^3$	NICS <sup>Iso</sup> (ppm)	CPU time (min)
PC <sub>60</sub> BM	6-31G(d)	2.19	2.84	-2.74	91	-1.5	585
	6-31+G(d,p)	2.14	2.81	-2.37	83	-1.4	1710

**Figure S1.** Structures of fullerene derivatives and corresponding experimental open-circuit voltage of P3HT:fullerene devices from Ref. [6].

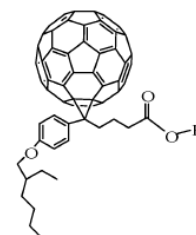
1) PC<sub>60</sub>BM ( $V_{OC}$ =600 mV)



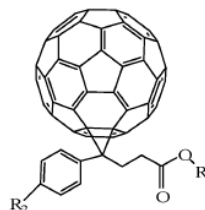
2) R=CH<sub>3</sub> ( $V_{OC}$  = 650 mV)



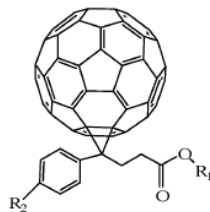
3) R=H ( $V_{OC}$  = 640 mV)



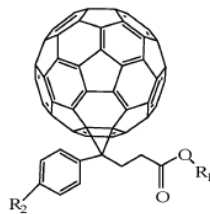
4) R<sub>1</sub>=CH<sub>3</sub>, R<sub>2</sub>=H ( $V_{OC}$  = 407 mV)



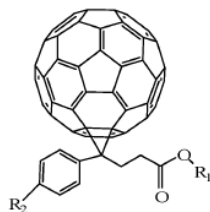
5)  $R_1=C_2H_5$ ,  $R_2=H$  ( $V_{OC} = 362$  mV)



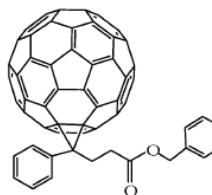
6)  $R_1= C_3H_9$ ,  $R_2=H$  ( $V_{OC} = 550$  mV)



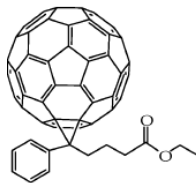
7)  $R_1=CH_3$ ,  $R_2=OCH_3$  ( $V_{OC} = 350$  mV)



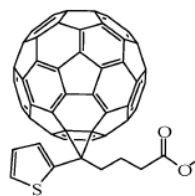
8) ( $V_{OC} = 580$  mV)



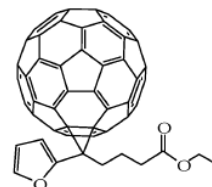
9) ( $V_{OC} = 640$  mV)



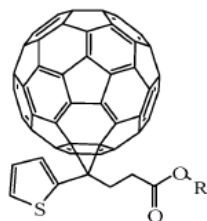
10 ( $V_{OC} = 600$  mV)



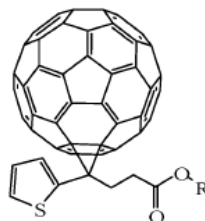
11 ( $V_{OC} = 600$  mV)



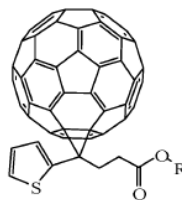
12) R=C<sub>2</sub>H<sub>5</sub> ( $V_{OC} = 600$  mV)



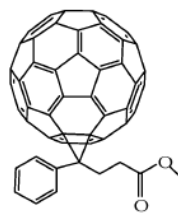
13) R=C<sub>3</sub>H<sub>9</sub> ( $V_{OC} = 600$  mV)



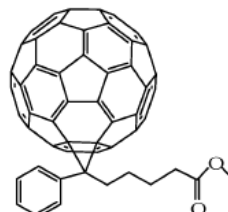
14) R=C<sub>4</sub>H<sub>9</sub> ( $V_{OC} = 600$  mV)



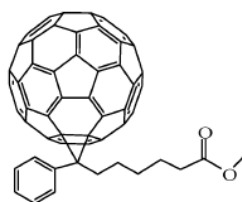
**15** ( $V_{OC} = 564$  mV)



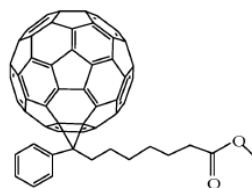
**16** ( $V_{OC} = 535$ )



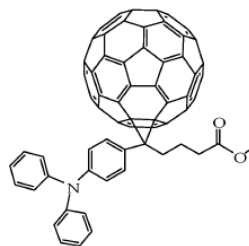
**17** ( $V_{OC} = 596$  mV)



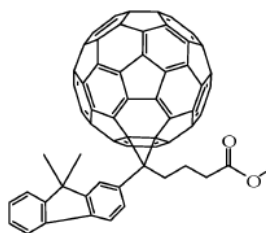
**18** ( $V_{OC} = 540$  mV)



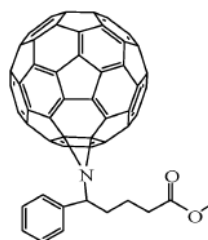
**19** ( $V_{OC} = 650$  mV)



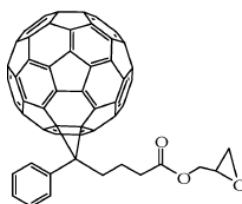
**20** ( $V_{OC} = 650$  mV)



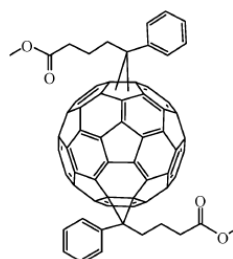
**21** ( $V_{OC} = 580$  mV)



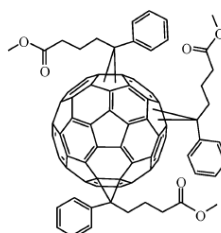
**22** ( $V_{OC} = 530$  mV)



**23** ( $V_{OC} = 730$  mV)



**24** ( $V_{OC} = 810$  mV)



25 ( $V_{OC} = 720$  mV)

