Theoretical Strategy To Design Novel n-Type Copolymers Based on Anthracene Diimide and Pyrido[2,3-g]quinoline Diimide for Organic Solar Cells

Zhiyong Fu, Wei Shen, Xiaoqin Tang, Min He, Rongxing He and Ming Li*

College of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, People's Republic of China

* **C**orresponding author. E-mail: liming@swu.edu.cn

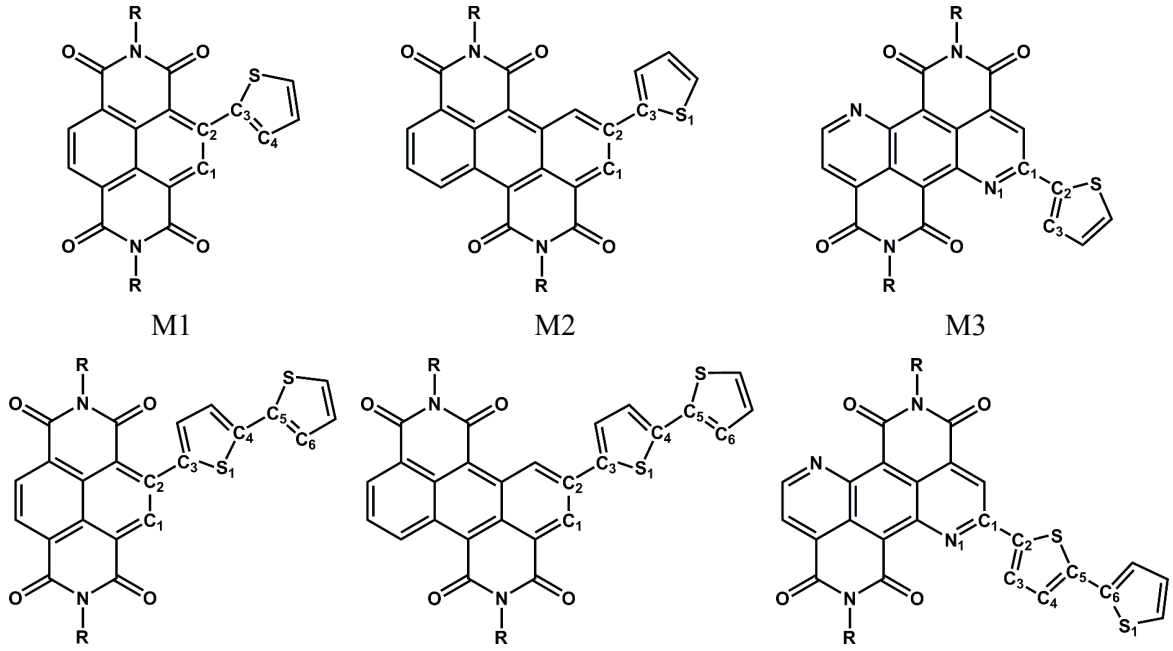
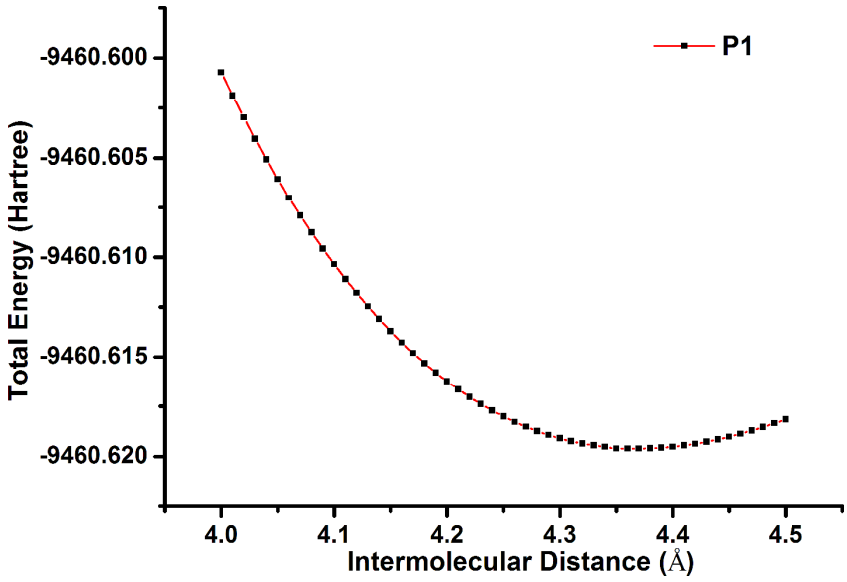
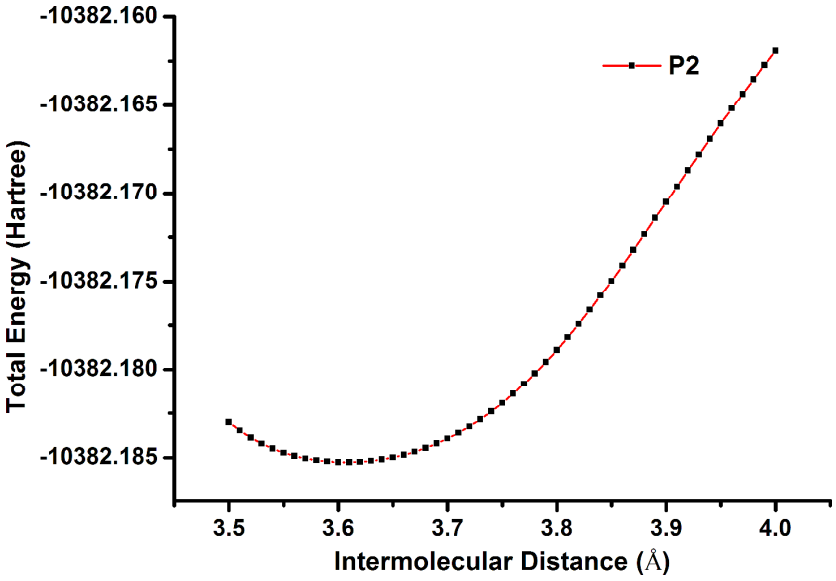


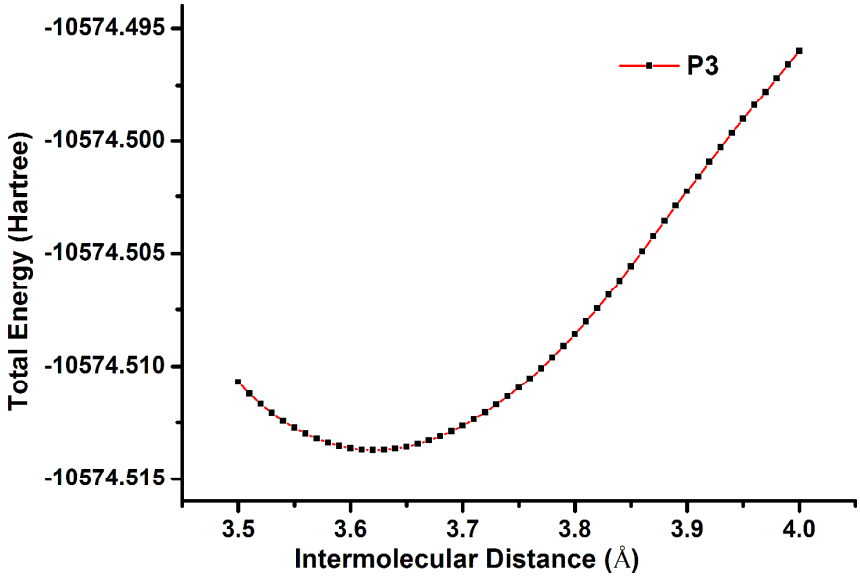
Figure S1. (a) Sketch structures (R = CH_3) and names of monomer models (M1-M3, M1a-M3a) and (b) 3D models of M1-M3, M1a-M3a.


P1
-9460.600
-9460.605
-9460.610
-9460.615
-9460.620
Total Energy (Hartree)
4.0
4.1
4.2
4.3
4.4
4.5
Intermolecular Distance (Å)

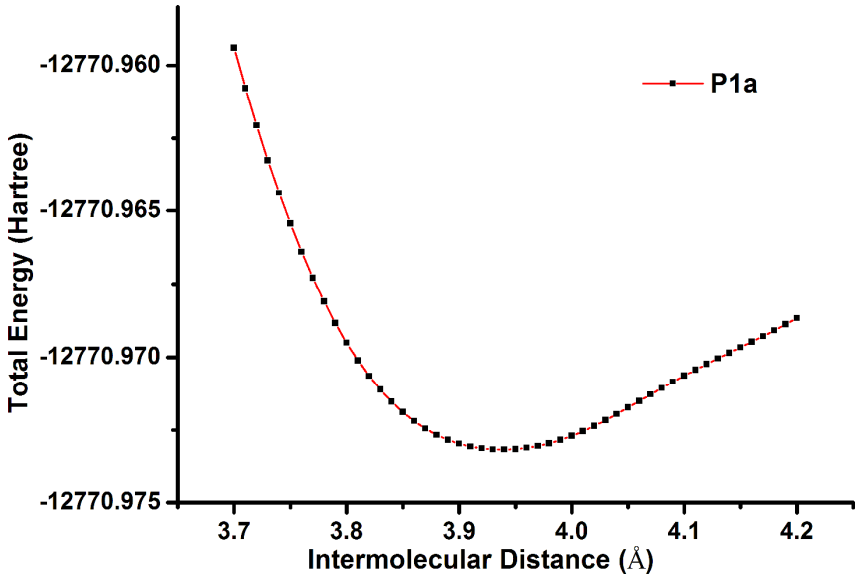
(a)


P2
-10382.160
-10382.165
-10382.170
-10382.175
-10382.180
-10382.185
Total Energy (Hartree)
3.5
3.6
3.7
3.8
3.9
4.0
Intermolecular Distance (Å)

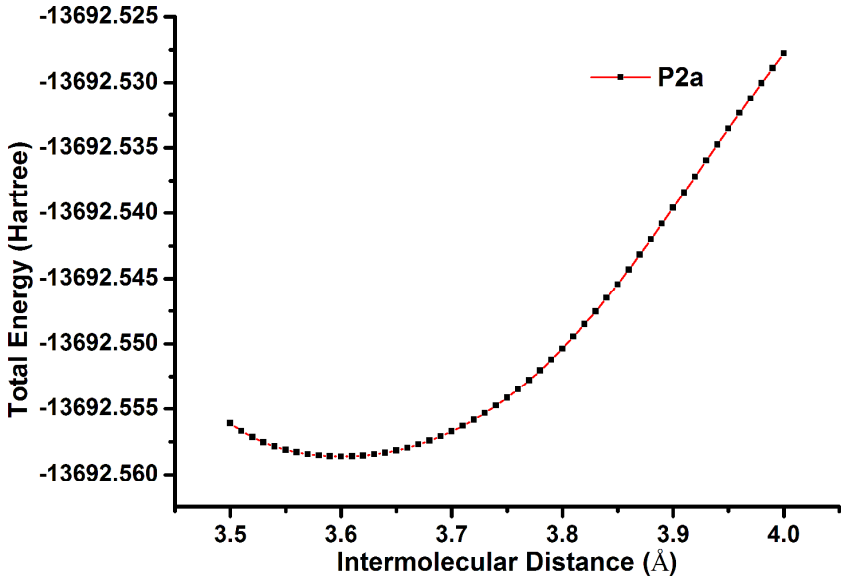
(b)


-10574.495
-10574.500
-10574.505
-10574.510
-10574.515
Total Energy (Hartree)
3.5
3.6
3.7
3.8
3.9
4.0
Intermolecular Distance (Å)
P3

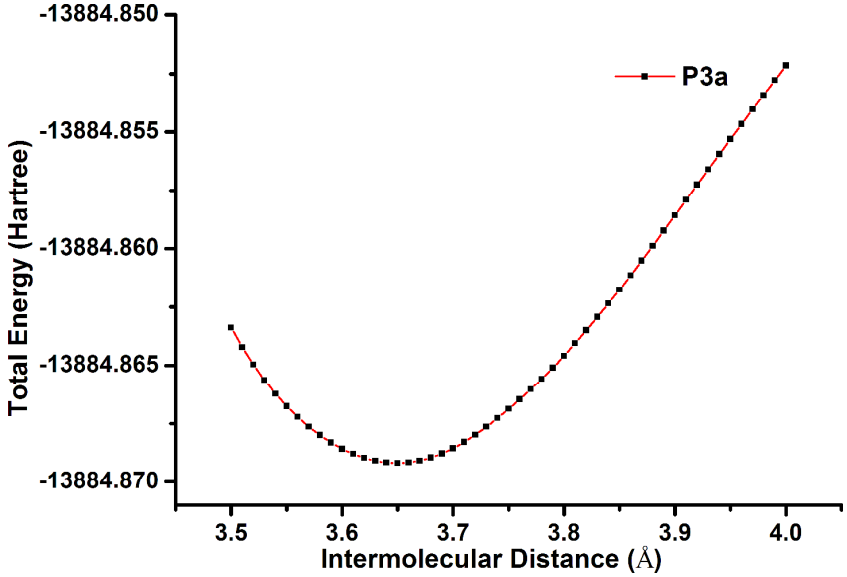
(c)


-12770.960
-12770.965
-12770.970
-12770.975
Total Energy (Hartree)
3.7
3.8
3.9
4.0
4.1
4.2
Intermolecular Distance (Å)
P1a

(d)



(e)



(f)

Figure S2. The calculated total energies of two adjacent trimers (P1 (a), P2 (b), P3 (c), P1a (d), P2a (e) and P3a (f)) as the function of intermolecular distance (scanning step length is 0.01 Å)

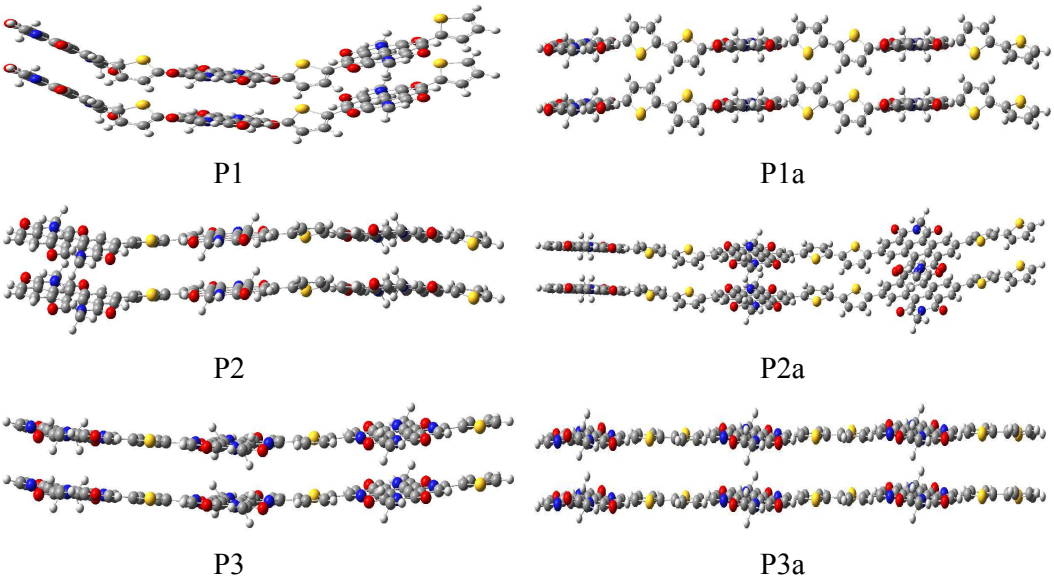


Figure S3. 3D models of two adjacent fragments of those copolymers