Supplementary Information for *Acta Phys. -Chim. Sin.*, 2010, 26(4): 1059-1064

二萘嵌苯二酰亚胺衍生物的半导体性质

蔡　雪[1,2]　　齐冬冬[1]　　张跃兴[1]　　边永忠[1]　　姜建壮[1,*]

([1]北京科技大学化学系, 北京　100083; [2]牡丹江师范学院化学系, 黑龙江 牡丹江　157012)

Semiconductor Properties of Perylene Diimide Derivatives

CAI Xue[1,2]　　QI Dong-Dong[1]　　ZHANG Yue-Xing[1]　　BIAN Yong-Zhong[1]　　JIANG Jian-Zhuang[1,*]

([1]*Department of Chemistry,University of Science and Technology Beijing, Beijing　100083, P. R. China;*

[2]*Department of Chemistry, Mudanjiang Normal College, Mudanjiang　157012, Heilongjiang Province, P. R. China*)

*Corresponding author.　Email: jianzhuang@ustb.edu.cn; Tel: +86-10-62332468.

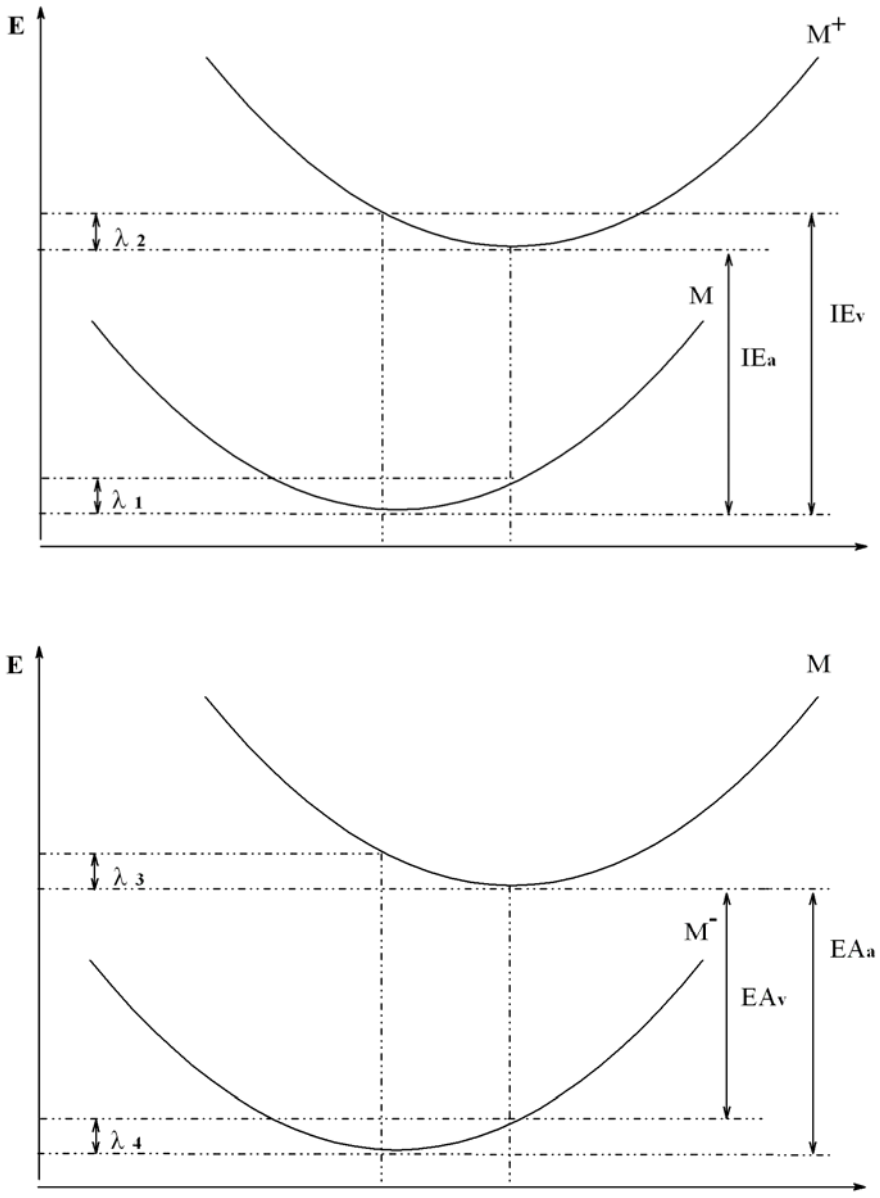

Fig.S1 Illustration of the internal reorganization energies of charge self-exchange process

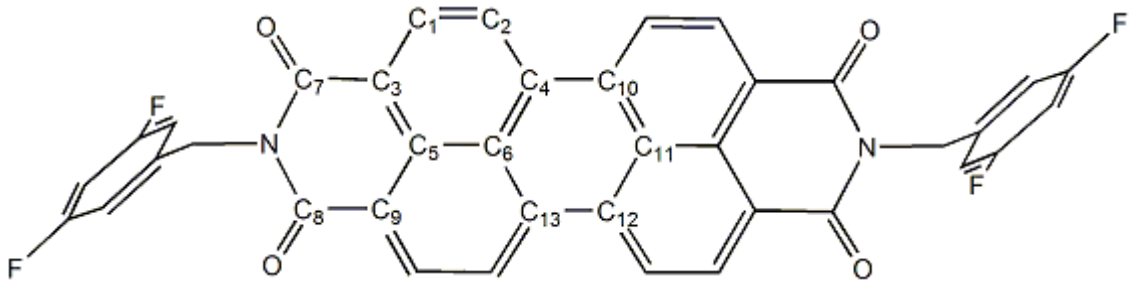

Fig.S2 Atom labels of 4

Table S1 B3lYP/6-31G(d) optimized geometries of neutral and anion of 4

parameter	Neutral (nm)	Anion (nm)
C_7-O	12.3668	12.2486
C_1-C_2	13.9874	13.8133
C_5-C_6	14.2923	14.5938
C_1-C_3	13.8426	14.0155
C_2-C_4	13.9648	14.1703
C_4-C_6	14.3124	14.3230
C_3-C_5	14.1599	14.1793
C_4-C_{10}	14.7049	14.4914
C_{10}-C_{11}	14.3129	14.3224
C_{11}-C_{12}	14.3124	14.3230
C_{12}-C_{13}	14.7049	14.4914
C_3-C_7	14.8187	14.5935
C-F	13.4829	13.5313
C_7-N	14.0863	14.0248