Electronic Supplementary Information

The interplay of intermolecular interactions, packing motifs and electron transport properties in perylene diimide related materials: A theoretical perspective

Yun Geng, Hai-Bin Li, Shui-Xing Wu and Zhong-Min Su*

Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun 130024, Peoples' Republic of China.

Author for correspondence: Prof. Zhong-Min Su, E-mail: zmsu@nenu.edu.cn.

Table S1 The crystal structures, the experimental electron mobilities (μ_{exp}) and their calculation values of all compounds listed in Fig. 1.

Compound	$\mu_{cal.}$ (cm^2/V.s)	$\mu_{exp.}$ [c] (cm^2/V.s)	Cell parameters (a, b, c in Å; α, β, γ in deg)	Ref.
1	—	—	4.87; 14.66; 10.84; 90; 91.33; 90	1
2	0.1 [a]	0.10 (Ref.1)	4.75; 8.48; 16.30; 86.88; 83.50; 83.68	2
3	—	1.7 (Ref. 3)	4.68; 8.50; 19.72; 85.99; 88.43; 82.79	4
4	0.37 [b]	0.72 (Ref.5)	4.91; 8.48; 16.29; 97.49; 94.37; 98.03	6
5	—	—	4.71; 15.00; 18.59; 109.72; 95.74; 92.82	7
6	—	—	21.23; 15.89; 6.93; 90; 90; 90	8
7	0.4 [a]	—	28.68; 4.47; 22.10; 90; 103.12; 90	9
8	0.5 [a]	—	4.26; 10.086; 17.346; 103.84; 92.42; 100.19	9
9	—	10.8 (Ref. 10)	5.23; 7.64; 18.82; 92.51; 95.25; 104.73	11
10	1.49 [b]	0.58 (Ref. 6)	17.46; 5.28; 15.28; 90; 110.897; 90	12
11	0.99 [b]	0.05 (Ref. 6)	9.20; 10.97; 14.92; 87.48; 88.09; 75.62	6
12	0.003 [b]	0.0005 (Ref. 6)	27.06; 7.07; 26.32; 90; 114.67; 90	6
13	0.025 [b]	0.0003 (Ref. 6)	27.86; 7.19; 13.01; 90; 115.18; 90	6
14	—	0.05 (Ref. 13)	11.60; 3.73; 28.06; 90; 96.65; 90	13
15	—	0.14 (Ref. 13)	4.95; 9.48; 13.06; 82.16; 81.68; 87.06	13
16	0.34 [b]	0.91 (Ref. 14)	14.46; 7.36; 20.03; 90; 90; 90	14

[a] Calculated electron mobilities in ref. 15. [b] Calculated electron mobilities in ref.16. [c] The experimental electron mobilities were measured in different OFET devices, please refer to the references listed in brackets for the detailed device data.

The electrostatic potential (ESP)

The electrostatic potential is given by the following expression:

$$V(\vec{r}) = \sum_{A} \frac{Z_A}{\left|\vec{r} - \vec{R}_A\right|} - \int \frac{\rho(\vec{r}')}{\left|\vec{r} - \vec{r}'\right|} d\vec{r}' \qquad \text{(S1)}$$

Where Z_A and $\vec{R}_A$ are the charge and position of nucleus A, respectively, and $\rho(\vec{r}')$ is the electron density at position $\vec{r}'$. The first term corresponds to the classical electrostatic potential of the nuclei and the second term corresponds to the quantum-mechanical electrostatic potential of the electrons. The sign of $V(\vec{r})$ indicates the relative dominant contribution coming from the positive nuclei or the negative electrons. When $V(\vec{r})$ mapped onto the molecular surface, namely $\rho(\vec{r}')$ = 0.001 au (electrons bohr^{-3}) contour and thus labeled as Vs(r), which could be used to analyze and predict the noncovalent interaction.[17]

References

1. K. Tojo and J. Z. Mizuguchi, Kristallogr. - New Cryst. Struct., 2002, 217, 45-46.
2. E. Hadicke and F. Graser, Acta Crystallogr., Sect. C: Cryst. Struct. Commun., 1986, 42, 189-195.
3. R. J. Chesterfield, J. C. McKeen, C. R. Newman, P. C. Ewbank, D. A. da Silva Filho, J.-L. Brédas, L. L. Miller, K. R. Mann and C. D. Frisbie, J. Phys. Chem. B, 2004, 108, 19281-19292.
4. A. L. Briseno, S. C. B. Mannsfeld, C. Reese, J. M. Hancock, Y. Xiong, S. A. Jenekhe, Z. Bao and Y. Xia, Nano Letters, 2007, 7, 2847-2853.
5. J. H. Oh, S. Liu, Z. Bao, R. Schmidt and F. Wurthner, Appl. Phys. Lett., 2007, 91, 212107-212103.
6. R. Schmidt, J. H. Oh, Y. S. Sun, M. Deppisch, A. M. Krause, K. Radacki, H. Braunschweig, M. Konemann, P. Erk, Z. A. Bao and F. Wurthner, J. Am. Chem. Soc., 2009, 131, 6215-6228.
7. G. Klebe, F. Graser, E. Hädicke and J. Berndt, Acta Crystallogr. Sect. B, 1989, 45, 69-77.
8. K. Hino, K. Sato, H. Takahashi, S. Suzuki and J. Mizuguchi, Acta Crystallogr. Sect. E, 2005, 61, o440-o441.
9. P. Zugenmaier, J. Duff and T. L. Bluhm, Cryst. Res. Technol., 2000, 35, 1095-1115.
10. N. A. Minder, S. Ono, Z. Chen, A. Facchetti and A. F. Morpurgo, Adv. Mater., 2012, 24, 503-508.
11. B. A. Jones, M. J. Ahrens, M.-H. Yoon, A. Facchetti, T. J. Marks and M. R. Wasielewski, Angew. Chem. Int. Ed., 2004, 43, 6363-6366.
12. R. Schmidt, M. M. Ling, J. H. Oh, M. Winkler, M. Konemann, Z. N. Bao and F. Wurthner,

Adv. Mater., 2007, 19, 3692-3695.

13. S. C. Martens, U. Zschieschang, H. Wadepohl, H. Klauk and L. H. Gade, Chem. -Eur. J., 2012, 18, 3498-3509.
14. M. Gsanger, J. H. Oh, M. Konemann, H. W. Hoffken, A. M. Krause, Z. N. Bao and F. Wurthner, Angew. Chem. Int. Ed., 2010, 49, 740-743.
15. M. C. R. Delgado, E. G. Kim, D. A. da Silva and J. L. Bredas, J. Am. Chem. Soc., 2010, 132, 3375-3387.
16. Y. Geng, J. Wang, S. Wu, H. Li, F. Yu, G. Yang, H. Gao and Z. Su, J. Mater. Chem., 2011, 21, 134-143.
17. F. Bulat, A. Toro-Labbé, T. Brinck, J. Murray and P. Politzer, J. Mol. Model., 2010, 16, 1679-1691.