Understanding Charge Transport Mechanisms in Organic Materials

Zhigang Shuai[1], Yuqian Jiang[2], Hua Geng[3] and Dong Wang[1]

[1]*Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China*
[2]*National Center for Nanoscience and Technology, Beijing 1000190, P. R. China*
[3]*Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China*
E-mail: zgshuai@tsinghua.edu.cn

We present our recent work on the understanding of the charge transport mechanism for organic optoelectronic materials, which has been under controversy. Semiclassical Marcus theory has been extremely popular and insightful for molecular design since Brédas and coworkers [1]. However, the experimental carrier mobility value of organic semiconductors increase rapidly in recent years to well exceed the theoretical limit based on Marcus theory, calling for improvement in computational method beyond the localized semiclassical limit. On the other hand, bandlike transport behavior has been observed for some ultra-pure and closely-packed organic single crystals [2]. We discuss about the effects of charge localization versus delocalization [3], quantum nuclear tunneling [4], dynamic disorder [5], bandlike versus impurity scattering [6], as well as superexchange effect in D-A mixed stacked crystal [7].

References

[1] Brédas J.L., Calbert J. P., da Silva Filho D. and Cornil J., *Proc. Natl. Acad. Sci. USA*, 99, (2002) 5804.
[2] Podzorov V., Menard E., Rogers J. A. and Gershenson M. E., *Phys. Rev. Lett.* 95, (2005), 226601.
[3] Jiang Y. Q., Zhong X.X., Shi W., Peng Q., Geng H., Zhao Y. and Shuai Z. G., *Nanoscale Horizons*, 1 (2016), 53-59.
[4] Geng H., Peng Q., Wang L. J., Li H. J., Liao Y., Ma Z. Y. and Shuai Z. G., *Adv. Mater.* 24, (2012), 3568-3572.
[5] Wang L. J., Li Q. K., Shuai Z. G., Chen L. P. and Shi Q., *Phys Chem Chem Phys* 12 (2010), 3309-3314.
[6] Shi W., Zhao T. Q., Xi J. Y., Wang D. and Shuai Z. G., *J. Am. Chem. Soc.* 137 (2015), 12929-12938.
[7] Geng H., Zheng X. Y., Shuai Z. G., Zhu L. Y. and Yi Y. P., *Adv. Mater.* 27 (2015) 1443-1449.