

# Effect of Biradical Character of Organic Molecules on Opto Electronic Properties

Ulrike Salzner

*Department of Chemistry, Bilkent University, Ankara, Turkey*

Most organic molecules and polymers used in organic electronics have closed-shell singlet ground states. Certain donor-acceptor systems, however, are open-shell singlet biradicals.<sup>[1]</sup> Presence of biradicals leads to close packing in crystals as intramolecular and intermolecular electron coupling compete with each other. As a result conductivity along stacking directions is particularly strong for crystals of biradicals.<sup>[2]</sup> Another important characteristic of biradicals is that they are prone to intramolecular singlet fission.<sup>[3]</sup> Singlet fission is a process during which the absorption of one photon leads to formation of two triplet states.<sup>[4]</sup> Intermolecular singlet fission was first observed in tetracene crystals<sup>[5]</sup> but in donor-acceptor systems<sup>[3]</sup> intramolecular singlet fission<sup>[6]</sup> has been demonstrated. Although direct formation of triplet states from singlet ground states is spin forbidden, quantum yields can reach almost 200%. In this presentation the effect of open-shell character of building blocks for organic electronics will be explored based on time-dependent density functional theory calculations.

- [1] a) M. Karikomi, C. Kitamura, S. Tanaka, Y. Yamashita, *J. Am. Chem. Soc.* **1995**, *117*, 6791-6792;  
b) U. Salzner, O. Karalti, S. Durdagi, *J. Mol. Model.* **2006**, *12*, 687-701.
- [2] J. D. Yuen, M. Wang, J. Fan, D. Sheberla, M. Kemei, N. Banerji, M. Scarongella, S. Valouch, T. Pho, R. Kumar, E. C. Chesnut, M. Bendikov, F. Wudl, *Journal of Polymer Science Part A: Polymer Chemistry* **2015**, *53*, 287-293.
- [3] E. Busby, J. Xia, Q. Wu, J. Z. Low, R. Song, J. R. Miller, X. Y. Zhu, L. M. Campos, M. Y. Sfeir, *Nat. Mater.* **2015**, *14*, 426-433.
- [4] M. B. Smith, J. Michl, *Chemical Reviews* **2010**, *110*, 6891-6936.
- [5] W. M. Moller, M. Pope, *The Journal of Chemical Physics* **1973**, *59*, 2760-2761.
- [6] E. G. Fuemmeler, S. N. Sanders, A. B. Pun, E. Kumarasamy, T. Zeng, K. Miyata, M. L. Steigerwald, X. Y. Zhu, M. Y. Sfeir, L. M. Campos, N. Ananth, *ACS Central Science* **2016**, *2*, 316-324.