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Bottom-up modelling of charge transport in polymer semiconductors DAVID CHEUNG, DAVID MCMAHON, ALESSANDRO TROISI, University of Warwick — By combining charge transport properties with ease of processing polymer semiconductors are attractive for large-area, low-cost applications, such as displays, or photovoltaics. Despite this interest, charge transport in polymers is poorly understood and, in particular, there is a gap between the phenomenological and microscopic descriptions of charge transport. In this presentation I will describe recent work that aims to bridge the divide between these levels of description. To explicitly consider both the nuclear and electronic degrees of freedom a combined molecular dynamics and quantum chemical study is performed on the archetypal polymer semiconductor, poly(3-hexylthiophene) (P3HT). MD simulations are used to generate configurations for quantum chemical calculations and to characterise the microstructure of P3HT[1]. The charge carriers become localized at long-lived traps[2]. The existence of activated transport is explained, and the trapped states are described with chemical detail. The charge transfer integrals, which are among the key parameters for charge transport models are calculated[1].

1. D. L. Cheung, D. P. McMahon, and A. Troisi, J. Phys. Chem. B, 113, 9393 (2009)
2. D. L. Cheung, D. P. McMahon, and A. Troisi, J. Amer. Chem. Soc., 131, 11179 (2009)

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