European XFEL Theory Seminar

Thursday, 16 March 2017, 17:00

Campus Schenefeld, main building (XHQ) room E1.173

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Charge transfer systems for molecular electronics

In the first part of my talk I will discuss the recently synthesized charge-transfer material picene–F4TCNQ [1], which can be used as a gate-voltage controlled molecular switch. We find switching ratios larger by one order of magnitude compared to an experimentally and theoretically well characterized anthraquinone based molecular system. Further, our calculations reveal that the picene–F4TCNQ system resembles remarkably well the I-V characteristics of a classical diode. The reverse-bias current of this molecular diode can be increased two orders of magnitude by an external gate voltage. Based on densityfunctional theory calculations we show that the hybrid states formed by the picene–F4TCNQ system play the key role in determining transport properties [2]. We further conclude that the tuning of quantum transport properties through hybrid states is a general concept which opens a new route towards functional materials for molecular electronics. In the second part of my talk I will focus on the correction of the self-interaction error that is inherent to all standard density functional theory calculations. Using the very recently developed Fermi-orbital based approach for the self-interaction correction by Pederson [3,4] we investigate systematically a set of different molecular systems ranging from simple diatomic to large organic molecules. We focus our analysis on the direct estimation of the ionization potential from orbital eigenvalues. Further, we show that the Fermi orbital positions in structurally similar molecules appear to be transferable [5].

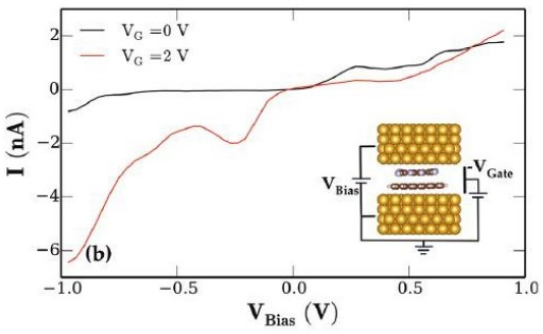
[1] B. Mahns, et al.: Crystal growth, structure, and transport properties of the chargetransfer salt Picene/2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane Cryst. Growth Des. 14 (2014) 1338 – 1346

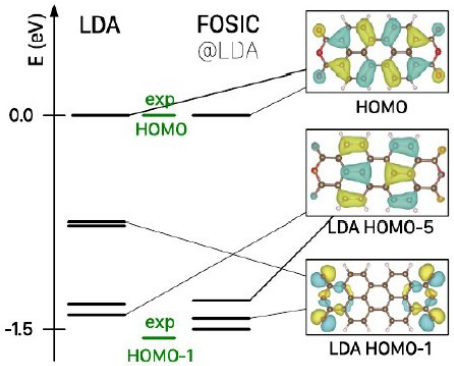
[2] T. Hahn, S. Liebing, J. Kortus: A gate controlled molecular switch based on picene–F4TCNQ charge-transfer material Nanoscale 6 (2014) 14508-14513

[3] M. R. Pederson et al.: J. Chem. Phys. 140, 121103 (2014)

[4] M. R. Pederson: J. Chem. Phys. 142, 064112 (2015)

[5] T. Hahn, S. Liebing, J. Kortus, M. R. Pederson: Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation J. Chem. Phys. 143 (2015) 224104





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