Effect of the electronic conjugation on the conductance of oligophenyl-derived molecules

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Using a density-functional-based transport method we study the conduction properties of several oligophenyl-derived dithiol (OPDDT) molecules wired to gold electrodes [1,2]. The OPDDT molecules differ in their side groups, which control the degree of conjugation of the π-electron system.
At first, we analyze the dependence of the low-bias zero-temperature conductance on the tilt angle between two phenyl ring units in biphenyl-derived molecules [2]. We show that the tilting of the phenyl rings results in a decrease of the low-bias conductance by roughly two orders of magnitude, when going from a planar configuration to a configuration in which the rings are perpendicular. Our findings are in good agreement with a recent experiment [3]. Additionally, we study the temperature dependence of both the conductance and its fluctuations and find qualitative differences between the analyzed molecular species.
Next, we investigate the length dependence of the conductance for three different families of OPDDT molecules, made up of between one and four phenyl rings [1]. For all the three families we observe an exponential decay of the conductance with respect to the length of the molecular wire. However, the attenuation factor is much larger for OPDDTs with a broken conjugation.

[1] F. Pauly, PhD thesis, Universität Karlsruhe, Karlsruhe (2007); S. Wohlthat, F. Pauly, J.K. Viljas, J.C. Cuevas, and G. Schön, arXiv:cond-mat/0702477.
[2] F. Pauly, J.K. Viljas, J.C. Cuevas, and G. Schön, arXiv:0705.3285 [cond-mat.mes-hall].
[3] L. Venkataraman et al., Nature **442**, 904 (2006).