

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Fullerene-based anchoring groups for molecular electronics: insights from theory ALEXEI BAGRETS, CHRISTIAN SEILER, VELIMIR MEDED, FERDINAND EVERS, Karlsruhe Institute of Technology – KIT, Germany. — Recent experiments [1] have explored the idea of using C60 as anchoring groups to increase the stability of single molecule junctions. To further explore this concept, we have performed elaborated electronic structure calculations based on the density functional theory. First, the influence of dispersive interactions on the location of C60 with respect to the electrode surface is carefully investigated. Second, the transmission of C60 and BDC60 [=1,4-bis(fullero[c]pyrrolidin-1-yl)benzene] junctions is obtained. We find that a mismatch of the chemical potential of Au electrodes and frontier molecular orbitals of C60 generates a tunneling barrier. As a consequence, BDC60 acts as a sequence of three weakly coupled quantum dots. Specifically, the small conductance values ($\sim 10^{-3} - 10^{-4} G_0$) observed experimentally [1], arise from the small broadening of the HOMO level of the inner molecule capped by C60 moieties. Third, electrode materials with a smaller work function (e.g. Ag instead of Au) are discussed, which might provide better matching to C60 and therefore establish more favorable conditions for electron transfer.

[1] C.A. Martin, D. Ding, J.K. Sørensen, T. Bjørnholm, J. van Ruitenbeek, H.S.J. van der Zant, JACS **130**, 13198-13199 (2008).

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Date submitted: 25 Nov 2009

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