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Electronic transport through alkane chains: the case of end group functionalization G. KIM, W. LU, S. WANG, M. BUONGIORNO NARDELLI, J. BERNHOLC, Dept. of Physics, NC State Univ. — Using first-principles calculations, we have investigated the mechanism of metal/molecule coupling and its influence on the electronic transport properties in the prototypical case of long hydrocarbon (alkane) chains sandwiched between gold contacts. In our study, 1-Pentanethiol [CH_3-$(CH_2)_4$- SH] , 1-Pentylamine [CH_3-$(CH_2)_4$-NH_2], octanediamine [$C_8H_{16}(NH_2)_2$] and octanedithiol [$C_8H_{16}(SH)_2$] are anchored to ideally terminated Au (111) surfaces in order to investigate the effects of the functionalization of the end groups on the conduction properties. The results indeed show that the end group functionalization plays a crucial role in controlling the electronic transport through the molecule: the effective contact resistance of the amine/Au system is much smaller than that of the thiol/Au one, giving rise to a large difference in the I-V characteristics. Our results are in good agreement with recent experimental measurements of the tunneling current through these functional groups [1].

[1] C. Chu and G. Parsons, to be published (2006)

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