Effects of molecular π-stacking on the conductance of nanographene-gold junctions

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First-principles calculations on several gold-acene-gold nanojunctions indicate that their low-bias conductance is due to the onset of a HOMO-derived resonance, thus being quite sensitive to the detailed interaction between the molecule and the gold leads. It is also found that such interaction is dominated by the electrophilic binding of Au to the acene, explaining the increase of the conductance as the ionization potential and the hardness of the molecular arrangement diminish. Both quantities are inversely proportional to the molecular length and the number of molecules present on a π stack, being also lower for circumacenes than for oligoacenes of the same size, opening a way to adjust the conductance by appropriate selection of the acene and control of its π-stacking. It is also found that the conductance depends dramatically on the amount of π overlap between the molecules in the stack, as well as on the particular disposition of the metallic tips with respect to the molecule. Calculations on charged nanojunctions of this type reveal their potential use as field-effect transistors. The conclusions reached point towards π-stacked arrangements of large circumacenes as potential candidates to build useful nanodevices for molecular electronics made out of nanographene-based materials.