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**Critical Roles of Metal-Molecule Contacts in Electron Transport Through Molecular-wire Junctions** ANTON GRIGORIEV, JONAS SKOLDBERG, GORAN WENDIN, MC2, Chalmers Univ of Technology, Gothenburg, Sweden, ZELJKO CRLJEN, Rudjer Boskovic Institute, Zagreb, Croatia — We use non-equilibrium Green's function DFT methods (TranSIESTA) to study the bonding-site dependence of the transmission through metal-molecule contacts in molecular junctions of type M-S-mol-S-M for a number of different molecular systems, mainly short molecules with DTB as a reference system, and also OPVn, n=3-5. For all systems on Au(111) surfaces the transmission is quite insensitive to the bonding site. However, if S is adsorbed in an Au vacancy, or on- top of a small (3-Au-atom) island, the transmission can drop very substantially due to mismatch and changes of the HOMO structure in the contacts. However, we do not find any examples of several orders-of-magnitude reductions of the conductivity. In several systems with low zero-bias transmission at the Fermi level, we found that buried Au-S contacts (S adsorbed in Au vacancy) are associated with very sharp LUMO levels just above the Fermi level. Such a system will show extremely strong non-linear effects and might work as uni- or bi-directional voltage-controlled 2-terminal switches.

Goran Wendin
MC2, Chalmers Univ of Technology, Gothenburg

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