Electronic and conducting properties of on N-heterocyclic carbenes on Au

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N-heterocyclic carbenes (NHCs) have attracted much attention recently as ligands for metal complexes and nanoparticles. NHCs are strong σ donors and were shown to have exceptional chemical and thermal stability on Au [1]. The binding of NHCs to Au is particularly interesting since electron transport through Au-C bonds was shown to be much higher than through any other metal-molecule link [2].

In this talk I will present results from Density-Functional Theory and Non-Equilibrium Green's Functions calculations for the electronic and transport properties of NHCs adsorbed on Au. First, I will address the adsorption structure of NHCs. I will then discuss the spectrum of NHC-terminated molecules, where we find a low-lying LUMO, whose position with respect to the Fermi level depends strongly on the atomistic termination of the metal-molecule contact. The LUMO position can be tuned by ~0.8 eV by the tip structure and this results in almost an order of magnitude modulation of conductance [3].

Finally I will address electron-vibration interaction and the stability of the junction under an applied voltage. Tunneling electrons can exchange energy with vibrations localized at the molecule. Energy released from electrons into vibrations causes the junction to heat, and could lead to its breakdown. Energy transferred from vibrational modes to the tunneling electrons is eventually released far away and so cools the junction. We calculate the rates of current-induced excitation or absorption of vibrations in NHC-based molecular junctions with different metal-molecule contacts. We find that, through the modulation of the interface electronic structure by the metal-molecule atomistic structure, the current can heat, but also cool, NHC-based junctions [4].

References:
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