Supporting Information

A comparative study of a triphenylene tricarbonyl chromium complex and its uncoordinated arene ligand on the Ag(111) surface: Influence of the complexation on the adsorption

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Molecular orbital plots of α-TPHC

In order to interpret the appearance of the complexes in the STM images, we performed quantum chemical calculations. Details of the calculation methods are given in the Experimental section of the manuscript. The following plots show the frontier orbitals (HOMO, HOMO-1, HOMO-2 and LUMO, LUMO+1, LUMO+2) of α-TPHC. The plots are accomplished with ORCA[1] through the interface to the gOpenMol[2] and Molekel[3] packages.

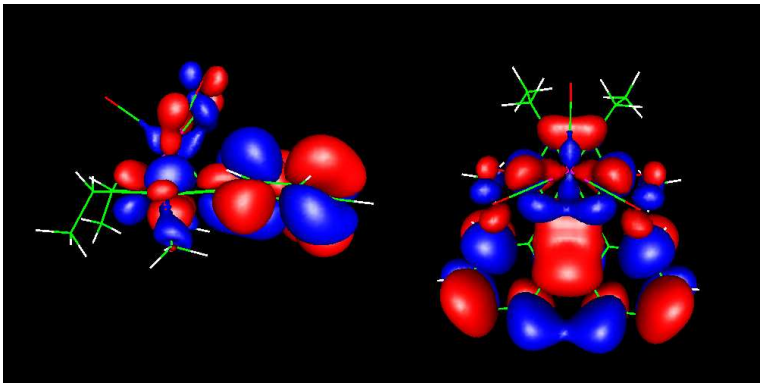

Figure 1: LUMO+2 of α-TPHC

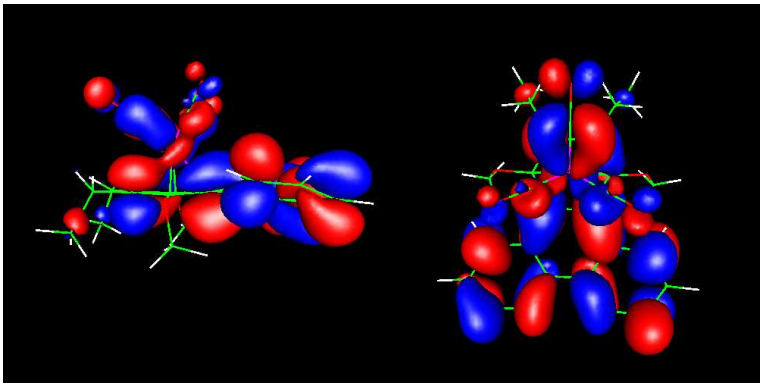

Figure 2: LUMO+1 of α-TPHC

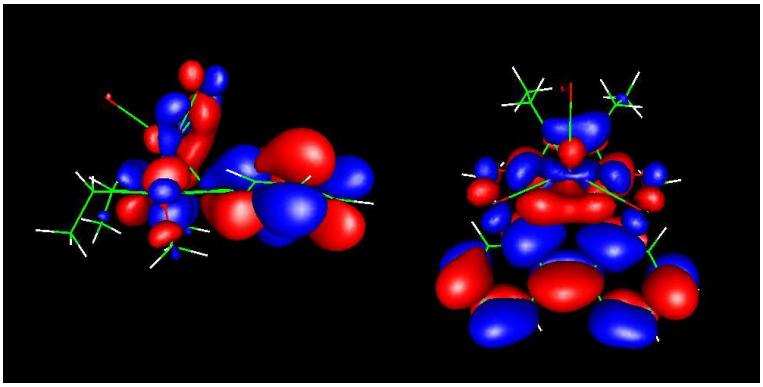

Figure 3: LUMO of α-TPHC

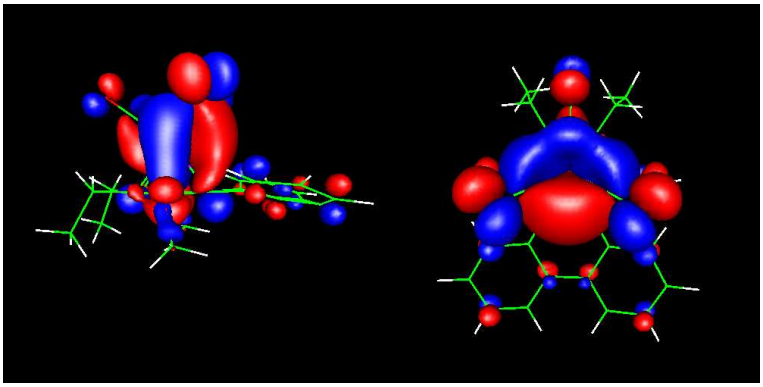

Figure 4: HOMO of α-TPHC

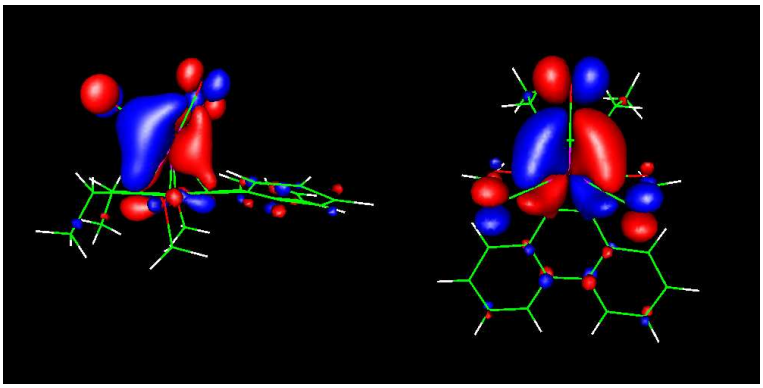

Figure 5: HOMO-1 of α-TPHC

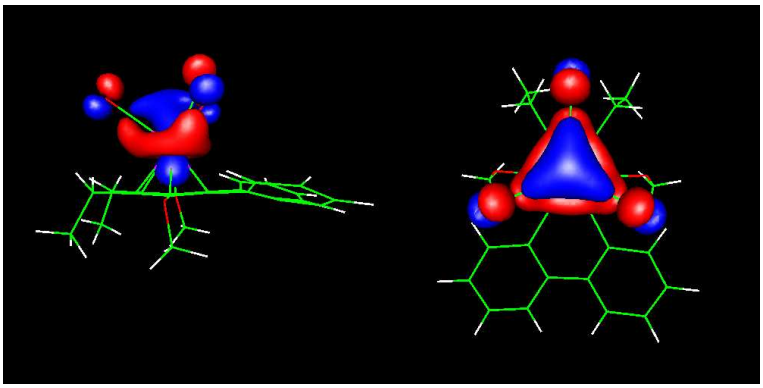

Figure 6: HOMO-2 of α-TPHC

References

(1) Neese, F., ORCA-an ab initio, Density Functional and Semiempirical Program Package, 2.5-20.2007; Universität Bonn; Bonn, Germany.

(2) http://laaksonen.csc.fi/gopenmol.

(3) http://www.cscs.ch/molekel/.