



Supporting Information

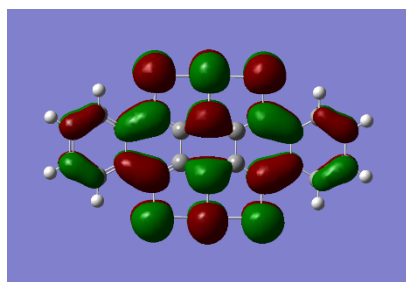
for

Pure and mixed ordered monolayers of tetracyano-2,6-naphthoquinodimethane and hexathiapentacene on the Ag(100) surface

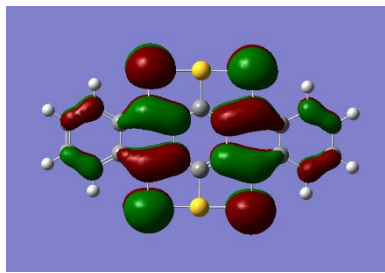
Robert Harbers, Timo Heepenstrick, Dmitrii F. Perepichka and Moritz Sokolowski

Beilstein J. Nanotechnol. **2019**, *10*, 1188–1199. [doi:10.3762/bjnano.10.118](https://doi.org/10.3762/bjnano.10.118)

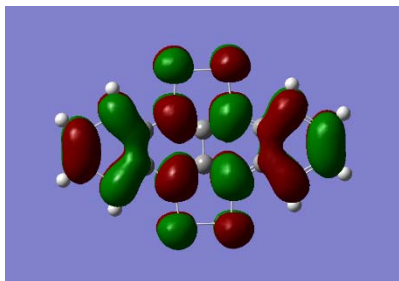
Frontier orbitals of molecules under study



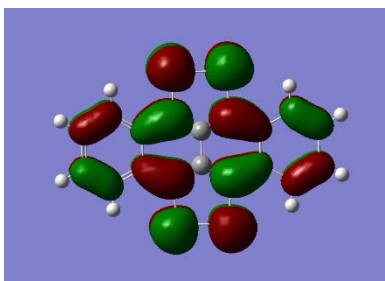
HTPEN LUMO = -3.28 eV



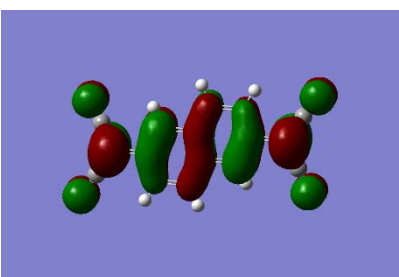
HTPEN HOMO = -5.38 eV



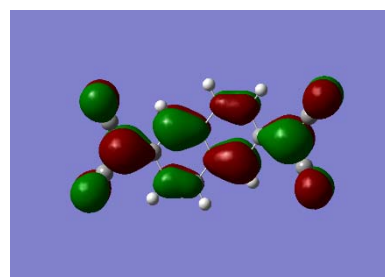
TTT LUMO = -2.37 eV



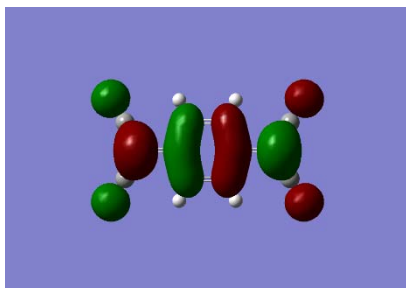
TTT HOMO = -4.39 eV



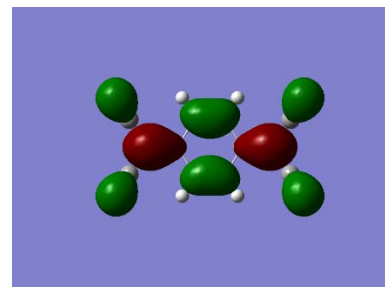
TNAP LUMO = -4.80 eV



TNAP HOMO = -6.75 eV



TCNQ LUMO = -4.82 eV



TCNQ HOMO = -6.74 eV

Figure S1: Frontier orbitals (LUMO and HOMO) and orbital energies of 5,6,7,12,13,14-hexathiapentacene (**HTPEN**), 5,6,11,12-tetrathiotetracene (**TTT**), 7,7,8,8-tetracyano-2,6-naphthoquinodimethane (**TNAP**) and 7,7,8,8-tetracyanoquinodimethane (**TCNQ**).