Supporting Information

Role of Organic Ligands Orientation on the Geometrical and Optical Properties of $Au_{25}(SCH_3)_{18}^0$

*Mirko Vanzan and Stefano Corni**

Department of Chemical Sciences, University of Padova, Via Marzolo 1, 35131 Padova, Italy

IR computed spectra of clusters A and B at the B3LYP//6-31G(d,p)/LANL2DZ geometry

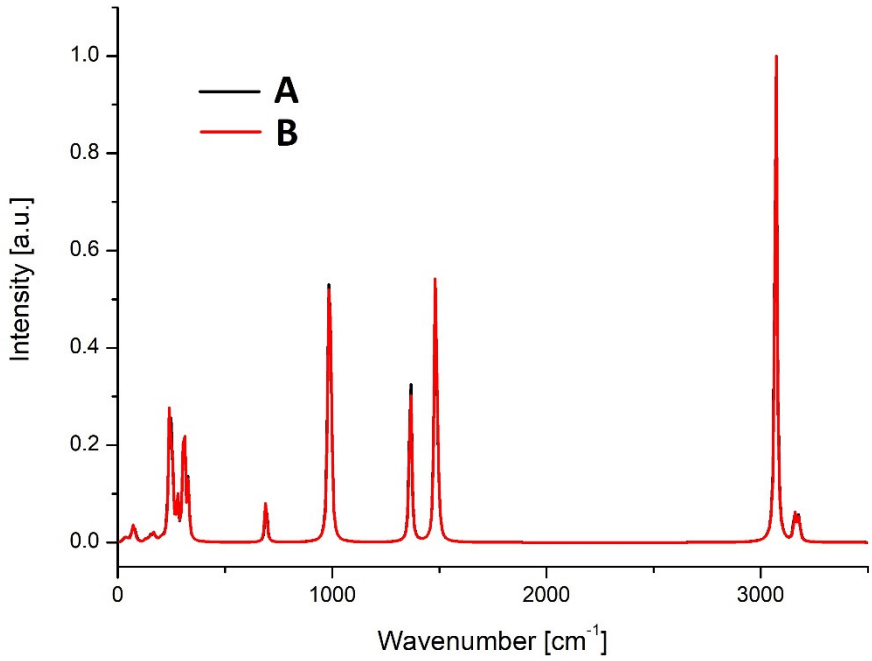

Figure S1. IR computed absorption spectra for clusters A and B calculated at the B3LYP//6-31G(d,p)/LANL2DZ geometry. Vibrational scaling factor = 1.0.

TDDFT computed spectrum of $Au_{25}(SCH_3)_{18}^0$ at the CAM-B3LYP//6-31G(d,p)/LANL2DZ level

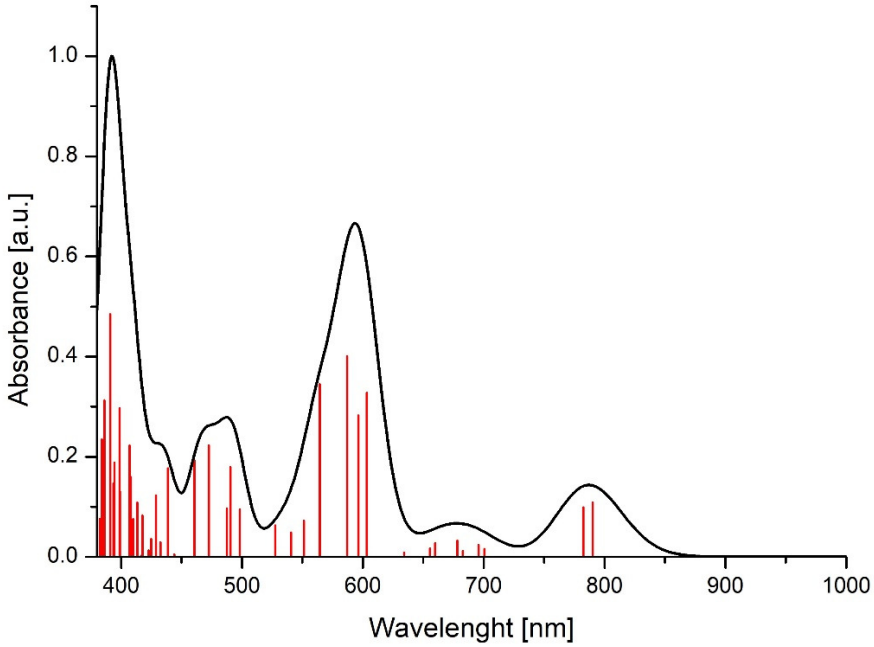

Figure S2. TDDFT computed absorption spectra for cluster B calculated at the CAM-B3LYP//6-31G(d,p)/LANL2DZ geometry. The original oscillator strengths are magnified by 10 times to ease their visualization.

The spectrum reported in Figure S2 presents several differences with respect to the ones reported in Figure 7. In particular there are two peaks (the major is around 600 nm and the minor is near 800 nm) which are not present in the experimental spectrum.

TDDFT computed spectrum of $Au_{25}(SCH_3)_{18}^0$ at the B3LYP//6-31G(d,p)/LANL2DZ level

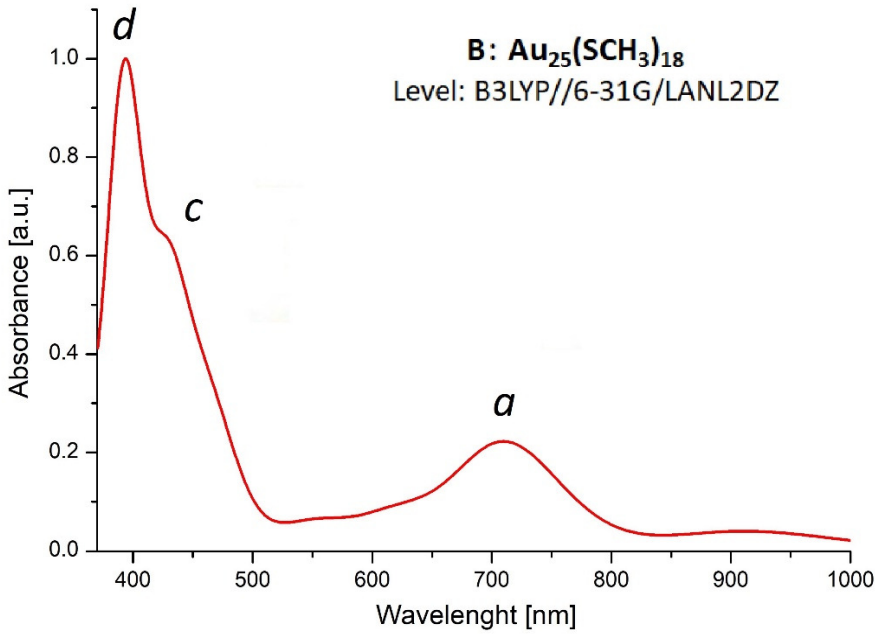

Figure S3. TDDFT computed absorption spectra for cluster B calculated at the CAM-B3LYP//6-31G(d,p)/LANL2DZ geometry. FWHM = 0.24 eV.

The spectrum reported in Figure S3 comes from the same TDDFT calculations as the one reported in Figure 6, but it is obtained by using a larger FWHM. The absorption profile is even closer to the experimental spectrum reported in Figure 7.