Supporting Information for:

Pd doping, conformational, and charge effects on the dichroic response of a monolayer protected Au_{38} nanocluster

Daniele Toffoli*, Oscar Baseggio, Giovanna Fronzoni, Mauro Stener*

Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste

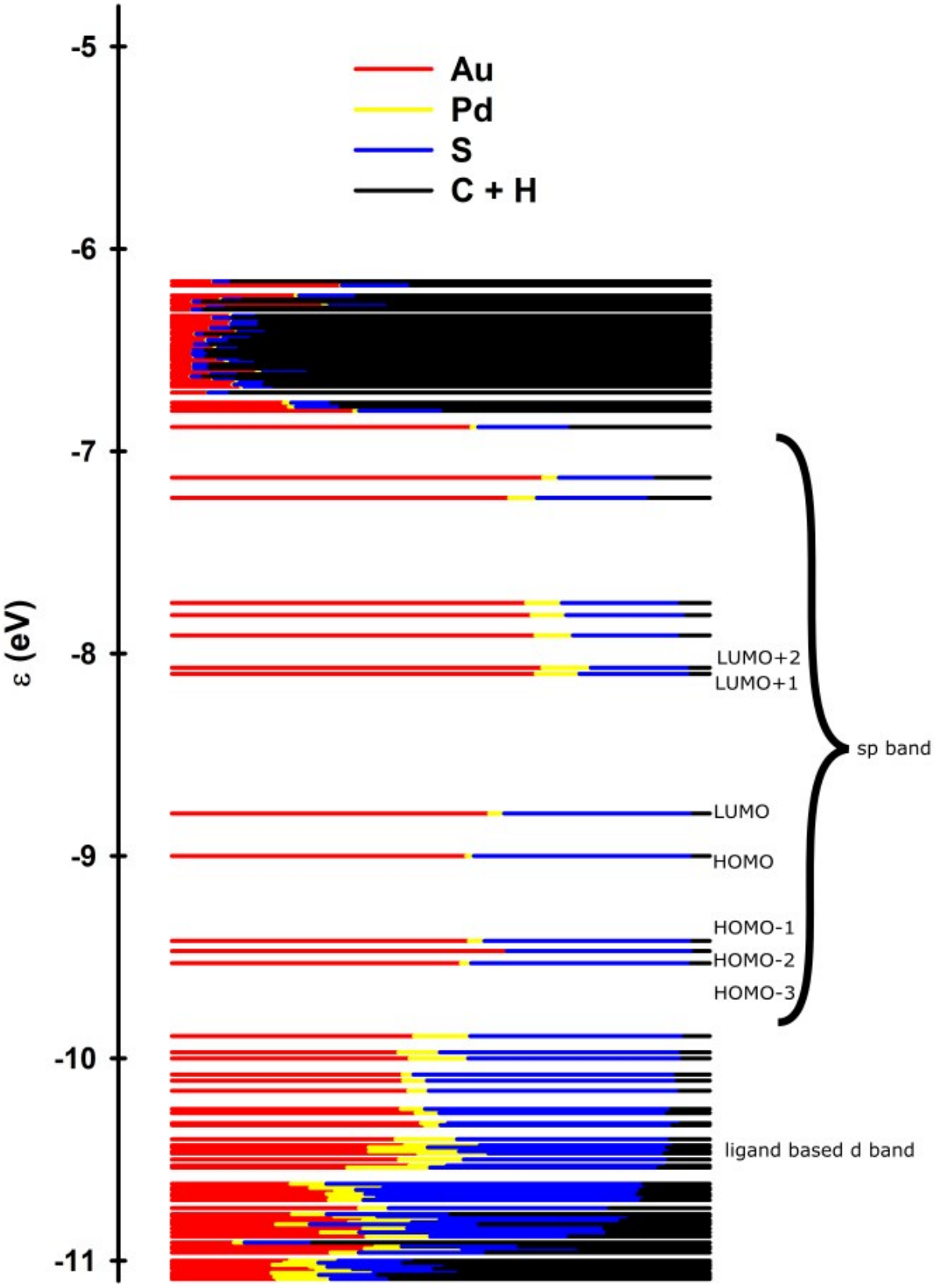
Via Giorgieri 1, 34127 Trieste, Italy

Alessandro Fortunelli* and Luca Sementa

CNR-ICCOM & IPCF, Consiglio Nazionale delle Ricerche

via Giuseppe Moruzzi 1, 56124, Pisa, Italia

*Authors to whom correspondence should be addressed, e-mail: toffoli@units.it, stener@units.it, alessandro.fortunelli@cnr.it



Scheme S1. Kohn-Sham energy-level diagram for $Au_{36}Pd_2(SCH_2CH_2Ph)_{24}$, geometry 1.

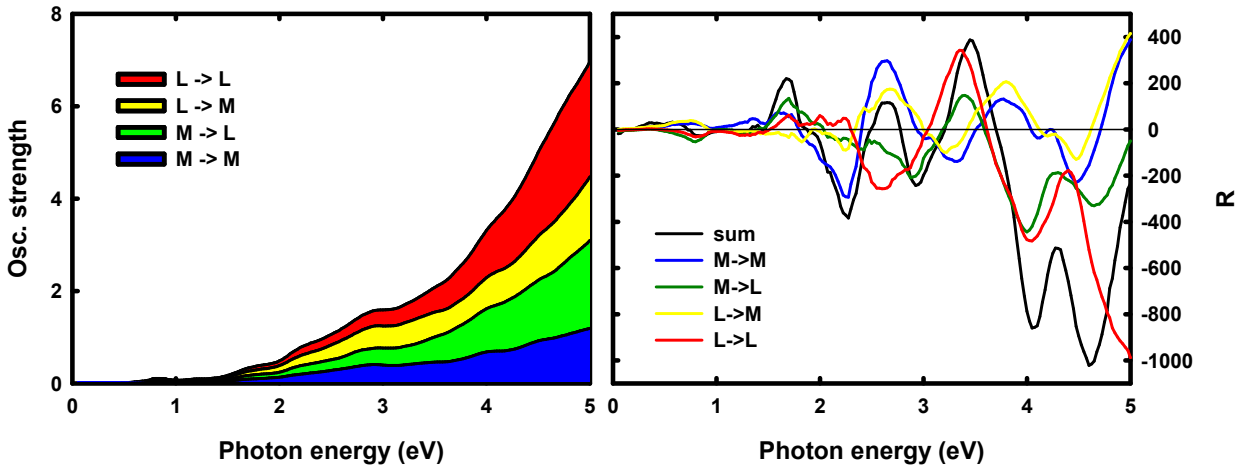


Figure S1. Fragment decomposition of the absorption spectrum (left panel) and of the CD spectrum for $Au_{36}Pd_2(SR)_{24}$, geometry 2. M=Au,Pd; L=S,C,H.

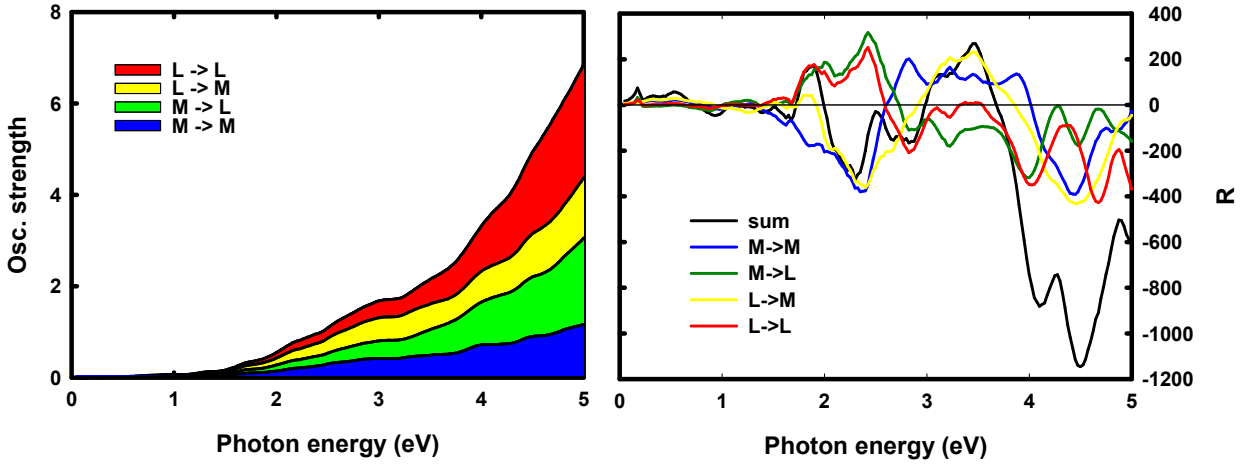


Figure S2. Fragment decomposition of the absorption spectrum (left panel) and of the CD spectrum for $Au_{36}Pd_2(SR)_{24}$, geometry 3. M=Au,Pd; L=S,C,H.

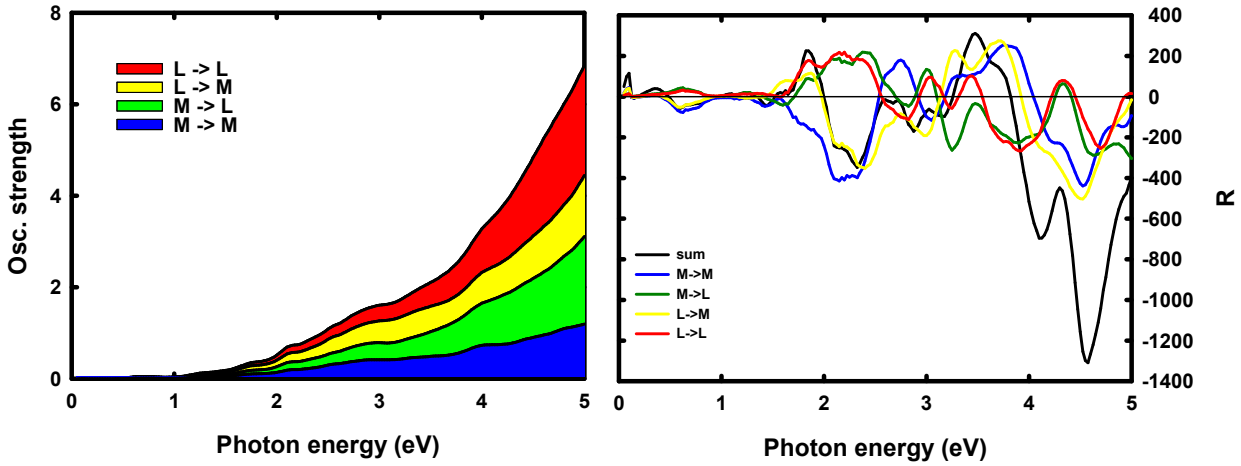


Figure S3. Fragment decomposition of the absorption spectrum (left panel) and of the CD spectrum for $Au_{36}Pd_2(SR)_{24}$, geometry 4. M=Au,Pd; L=S,C,H.

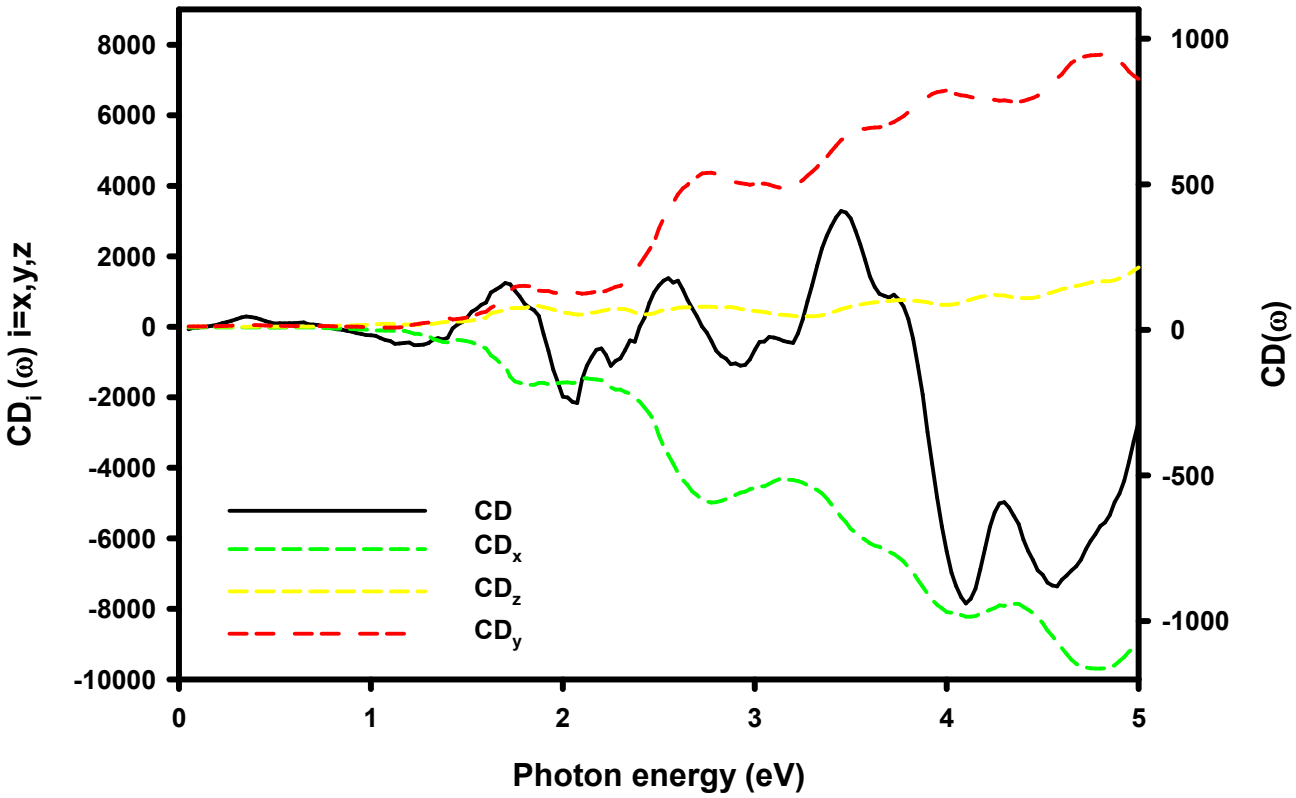


Figure S4. Decomposition of the CD spectrum of the $Au_{36}Pd_2(SR)_{24}$ cluster, geometry **1**, into its *x*- *y*- *z*- cartesian components. Rotatory strengths are in units of 10^{-40} esu^2 cm^2.

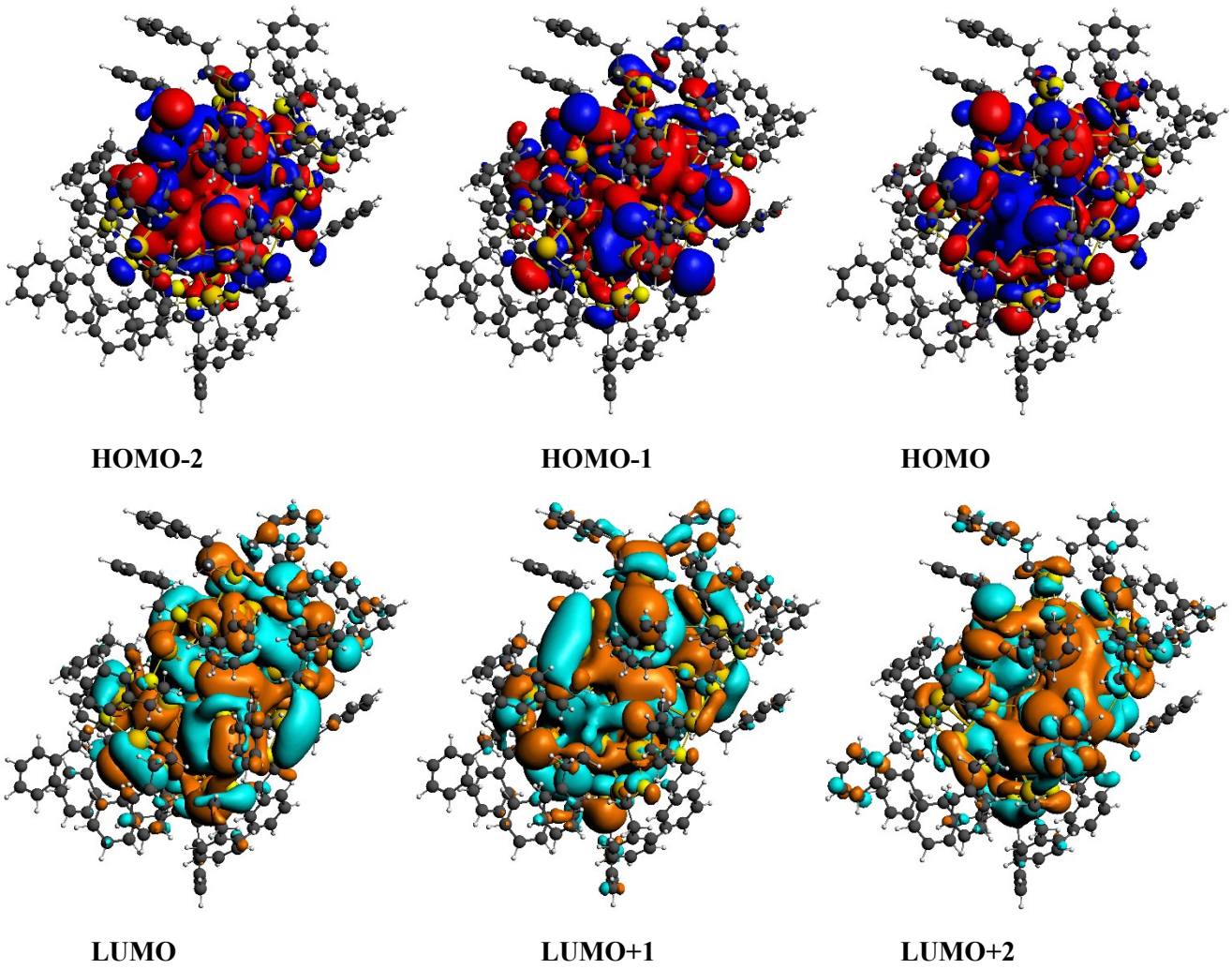
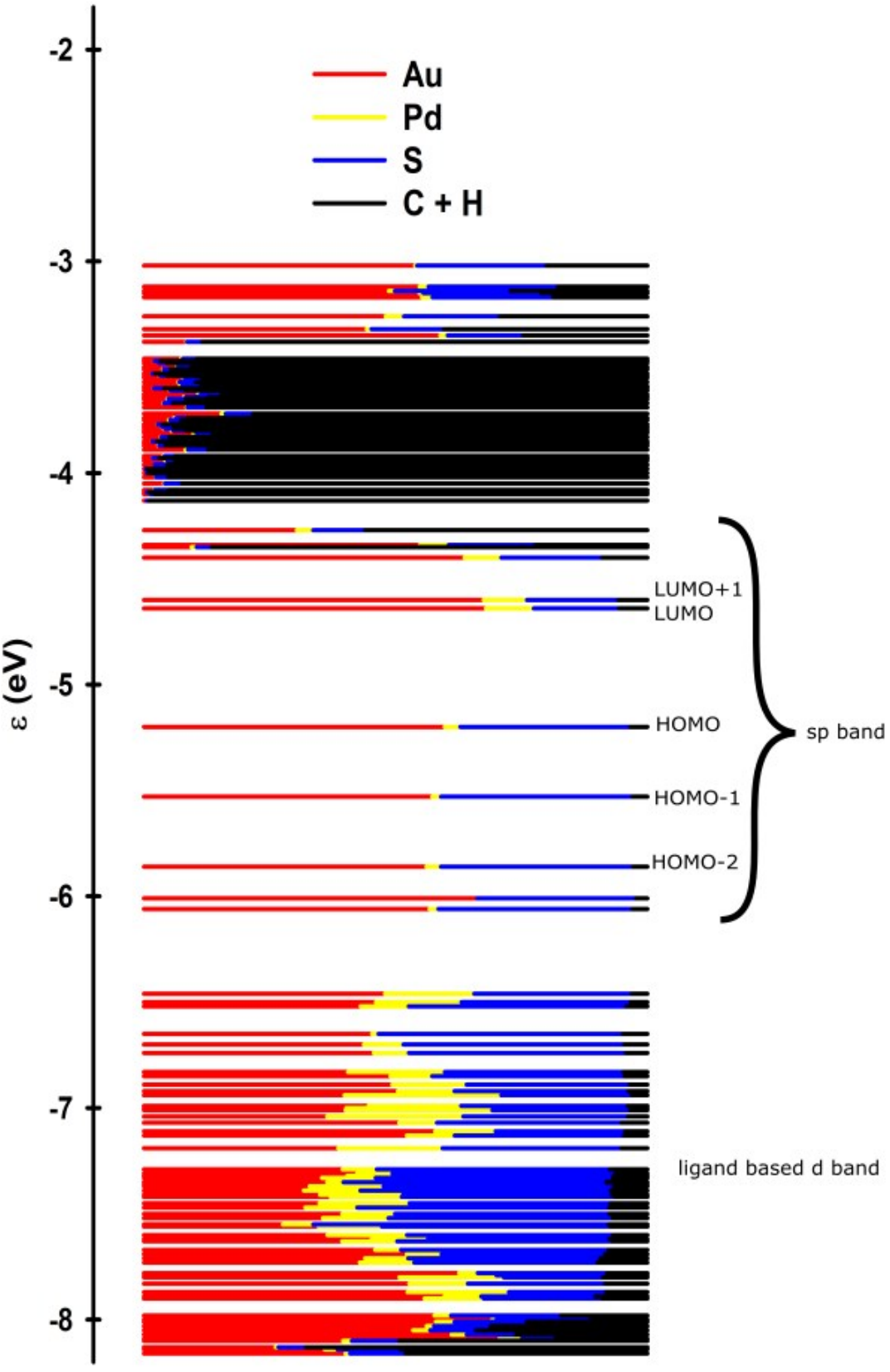


Figure S5. Plot of selected Kohn-Sham MOs of $Au_{36}Pd_2(SC_2H_4Ph)_{24}^{2-}$, geometry 1. Orbitals are plotted with the ADFview program, using a contour value of 0.005 bohr $^{-3/2}$.



Scheme S2. Kohn-Sham energy-level diagram for $Au_{36}Pd_2(SCH_2CH_2Ph)_{24}^{2-}$, geometry 1.

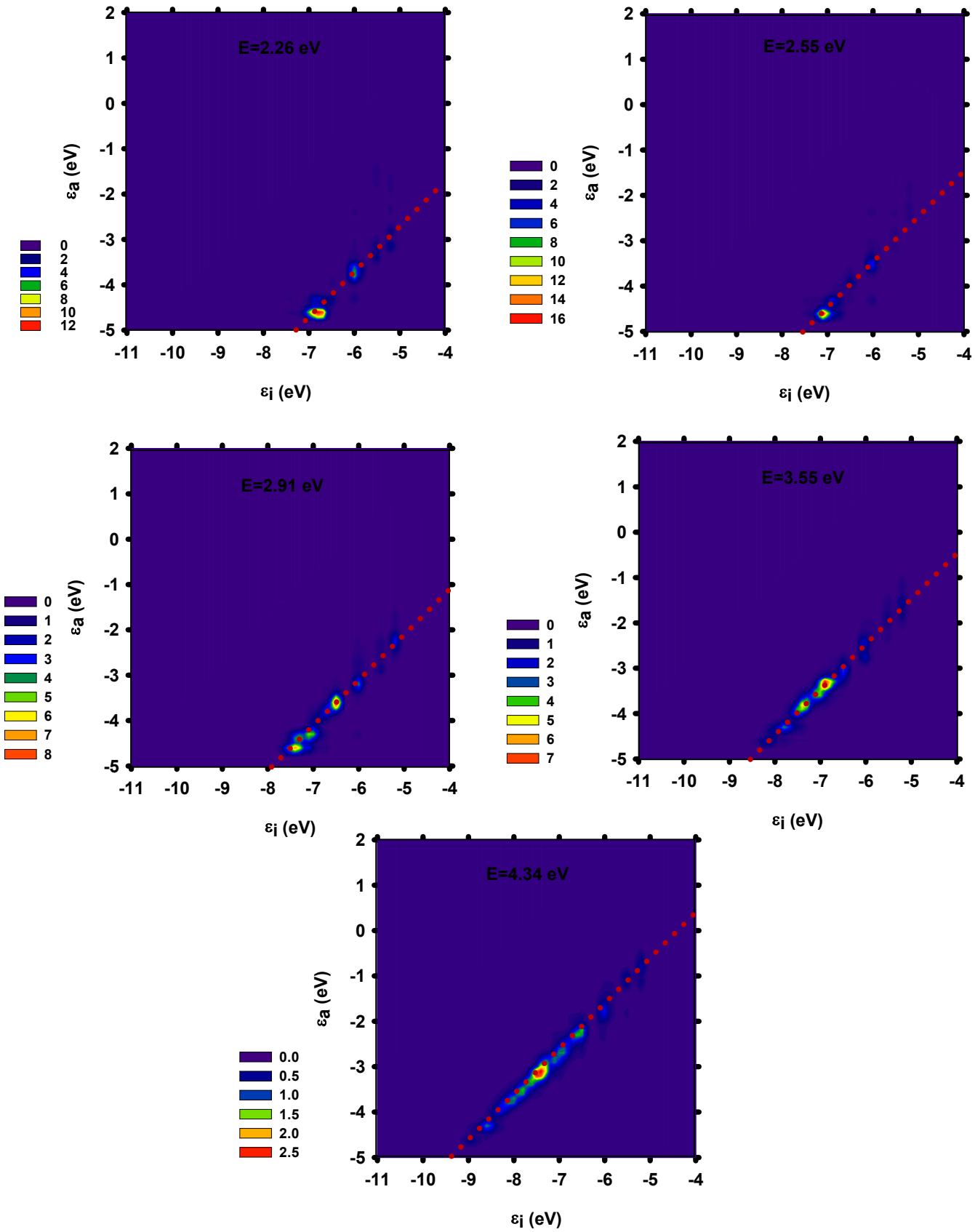


Figure S6. TCM analysis of $Au_{36}Pd_2(SC_2H_4Ph)_{24}^{2-}$, geometry **1**, at selected excitation energies. *X* and *Y* axes refer to KS occupied and virtual orbitals respectively. Dotted lines obey the equation $\epsilon_a - \epsilon_i = \omega$, where ω is the photon energy.

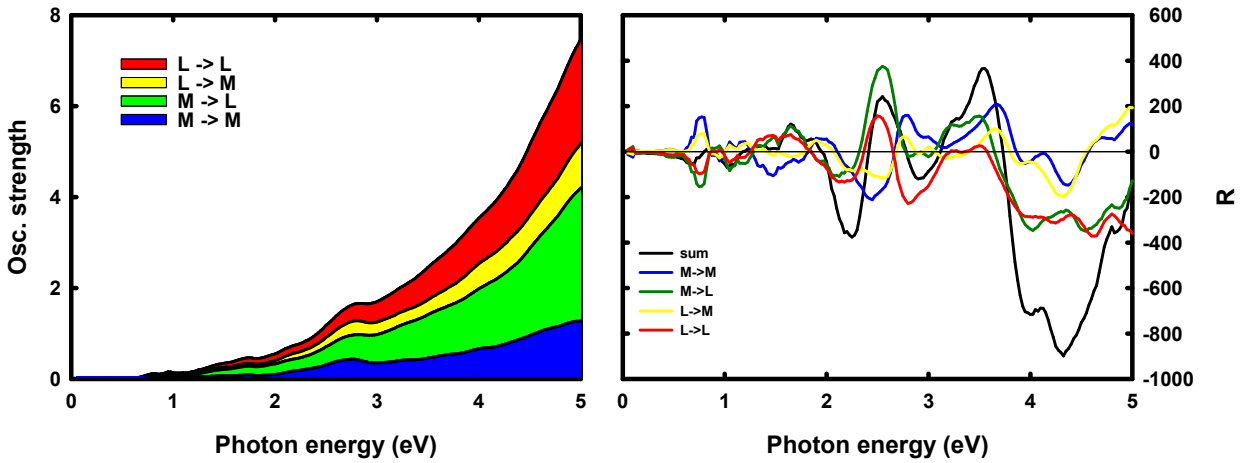


Figure S7. Fragment decomposition of the absorption spectrum (left panel) and of the CD spectrum for $Au_{36}Pd_2(SR)_{24}^{2-}$, geometry 1. M=Au,Pd; L=S,C,H.

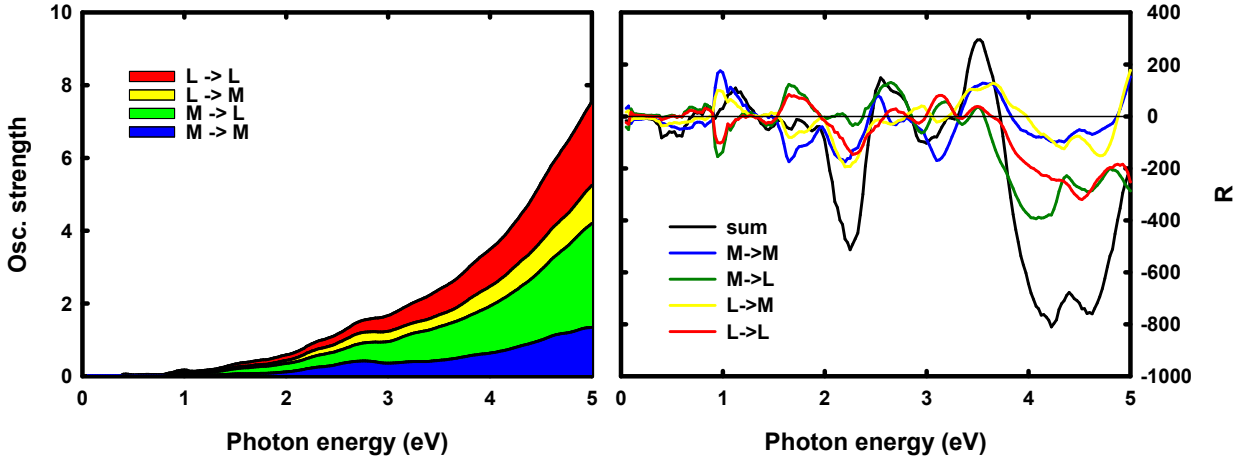


Figure S8. Fragment decomposition of the absorption spectrum (left panel) and of the CD spectrum for $Au_{36}Pd_2(SR)_{24}^{2-}$, geometry 2. M=Au,Pd; L=S,C,H.

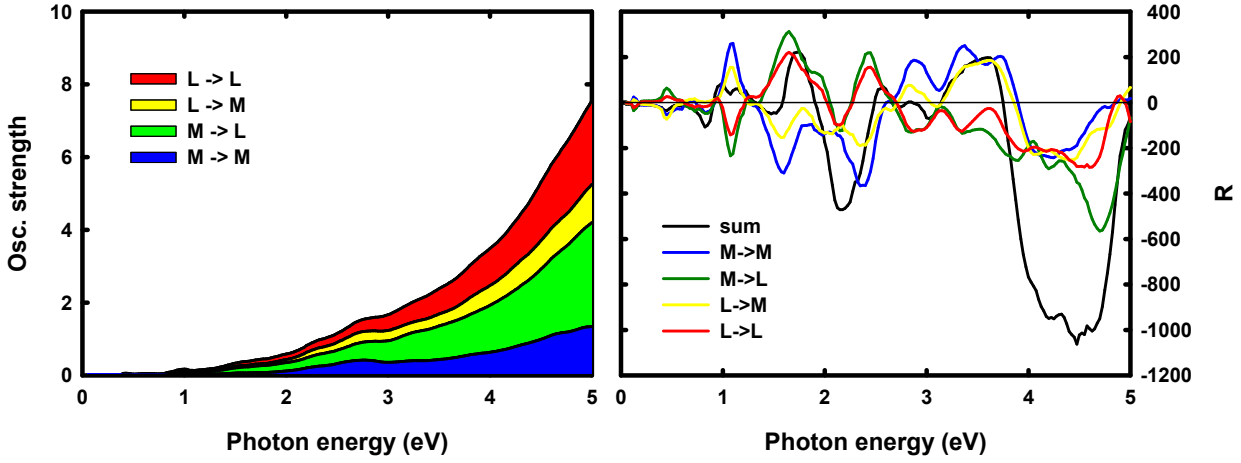


Figure S9. Fragment decomposition of the absorption spectrum (left panel) and of the CD spectrum for $Au_{36}Pd_2(SR)_{24}^{2-}$, geometry 3. M=Au,Pd; L=S,C,H.

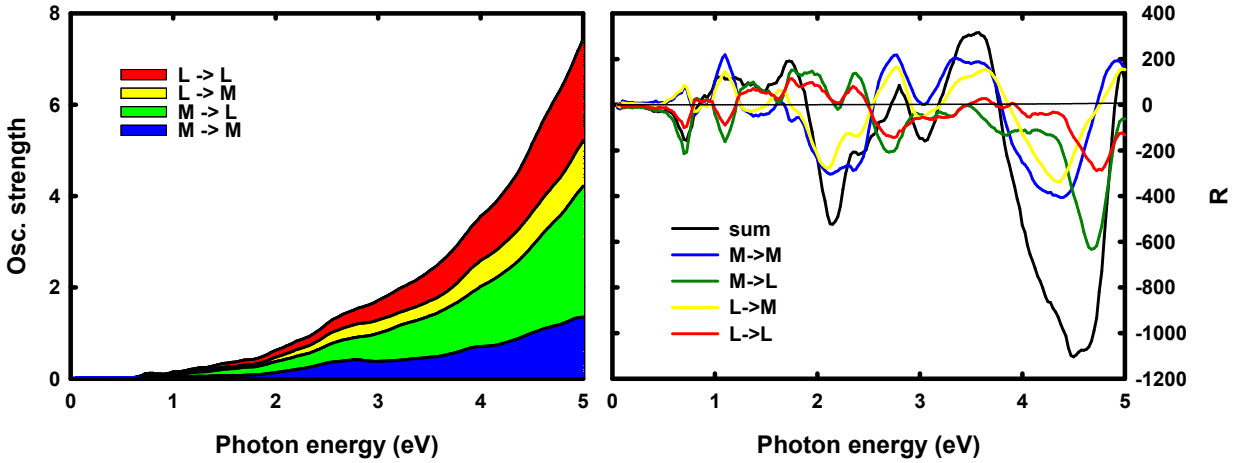


Figure S10. Fragment decomposition of the absorption spectrum (left panel) and of the CD spectrum for $Au_{36}Pd_2(SR)_{24}^{2-}$, geometry 4. M=Au,Pd; L=S,C,H.