Supporting Information for:

**Pd doping, conformational, and charge effects on the dichroic response of a monolayer protected Au$_{38}$ nanocluster**

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Scheme S1. Kohn-Sham energy-level diagram for Au$_{36}$Pd$_2$(SCH$_2$CH$_2$Ph)$_{24}$, 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$_2$CH$_2$Ph)$_{24}^{2-}$, geometry 1.
Figure S6. TCM analysis of \( \text{Au}_{36}\text{Pd}_2(\text{SC}_2\text{H}_4\text{Ph})_{24}^{2-} \), 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 \( \omega \) 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.