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Supplementary Information:Computational investigation of CO adsorbed on Au_x, Ag_x and $(AuAg)_x$ nanoclusters (x = 1-5, 147)and monometallic Au and Ag low-energy surfaces

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Table S1. Influence of spin configuration on the energy (E_{+CO}^{DFT}) of Au_5CO, Au_3CO, $Au(CO)_2$ and AuCO, in eV. ΔE_{SUP+CO}^{DFT} is also given, in eV, defined as the difference in energy between the lowest energy spin-configuration for a given composition, highlighted in grey, and the energy of the system being modelled.

Structure	**Spin state (μ)**	E_{SUP+CO}^{DFT}	$\mathbf{\Delta}E_{SUP+CO}^{DFT}$
Au_5CO	3	−23.644	2.02
Au_5CO	2	−24.693	0.97
Au_5CO	1	−25.663	0.00
Au_5CO	0	−25.643	0.02
Au_3CO	3	−18.497	2.63
Au_3CO	2	−19.709	1.42
Au_3CO	1	−21.132	0.00
Au_3CO	0	−21.114	0.02
$Au(CO)_2$	1	−32.650	0.00
$Au(CO)_2$	0	−32.644	0.01
Au(CO)	1	−16.301	0.00
Au(CO)	0	−16.296	0.00