Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Superatomic and adsorption properties of Ni atom doped Au clusters

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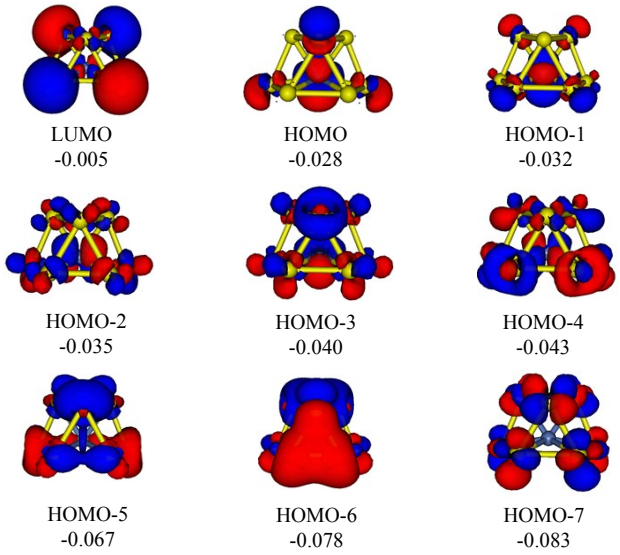

Fig. S1 The molecular orbital diagrams and orbital energies (a.u) of the $NiAu_7^-$ cluster.

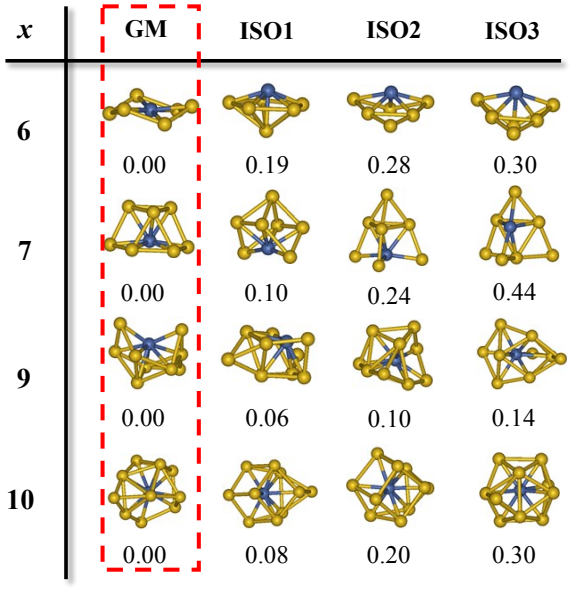

Fig. S2 Optimized isomers and relative stabilities (eV) of $NiAu_n$ (n=6-10).

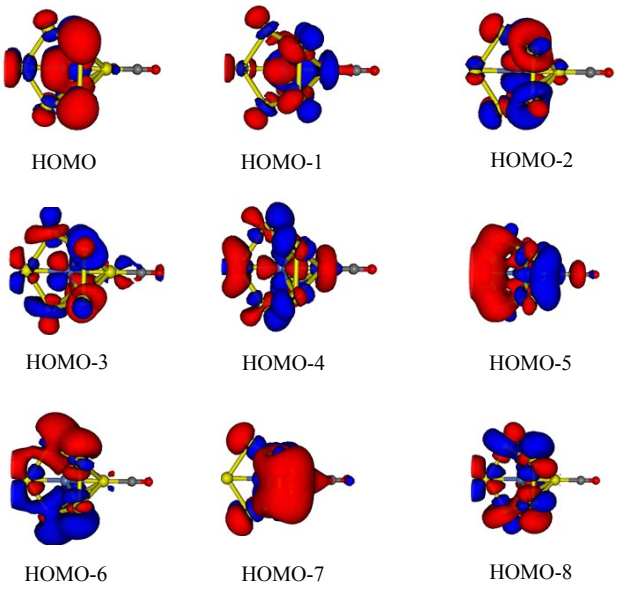

Fig. S3 The molecular orbital diagrams of the $NiAu_8$-CO structure.

Table S1. The embedding energies (*EE*, eV) of the Ni atom within Au clusters according to: $EE = E(Au_x) + E(Ni) - E(NiAu_x)$

x	$NiAu_7^-$	$NiAu_8$	$NiAu_9^+$
EE (eV)	3.11	3.26	3.64

Table S2. The adiabatic ionization potential (E_{AIP}), adiabatic electron affinity (E_{AEA}) and HOMO-LUMO gaps (E_{HL}) of the alloy clusters.

x	$NiAu_7^-$	$NiAu_8$	$NiAu_9^+$
E_{AIP} (eV)		6.86	6.00
E_{AEA} (eV)	2.51	2.26	
E_{HL} (eV)	0.64	1.11	0.83