Supporting Information:

Table SI-1: Interaction energy (kcal/mol) of pristine and doped gold clusters with CO, obtained by M06 method, for different cluster sizes.

Cluster size (*n*)	Au_nCO	$Au_{n-1}HCO$	$Au_{n-1}LiCO$	$Au_{n-1}NaCO$
2	-23.30	-24.88	-7.35	-3.82
3	-28.31	-21.80	-9.86	-6.66
4	-24.00	-24.17	-9.92	-6.91
5	-16.29	-20.87	-9.55	-6.76
6	-13.27	-11.15	-9.89	-9.54
7	-15.93	-22.84	-13.64	-8.99
8	-11.82	-21.12	-10.91	-10.26

FIGURE CAPTIONS

Figure SI-1: Optimized geometries of pristine and doped gold clusters obtained by using M06 method.

Figure SI-2: Optimized geometries of CO-adsorbed pristine and doped gold clusters obtained with M06 method.

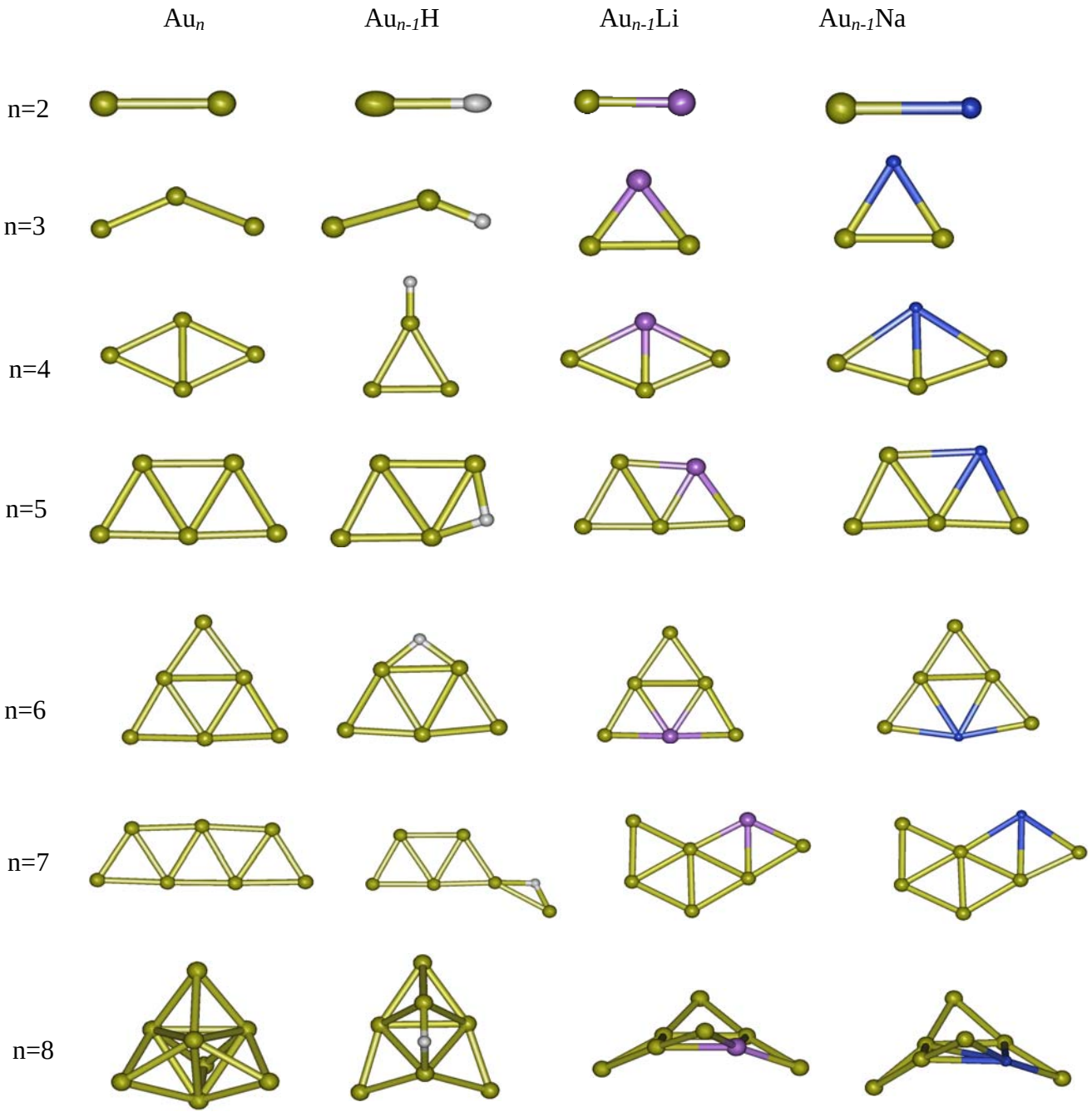

Figure SI-1

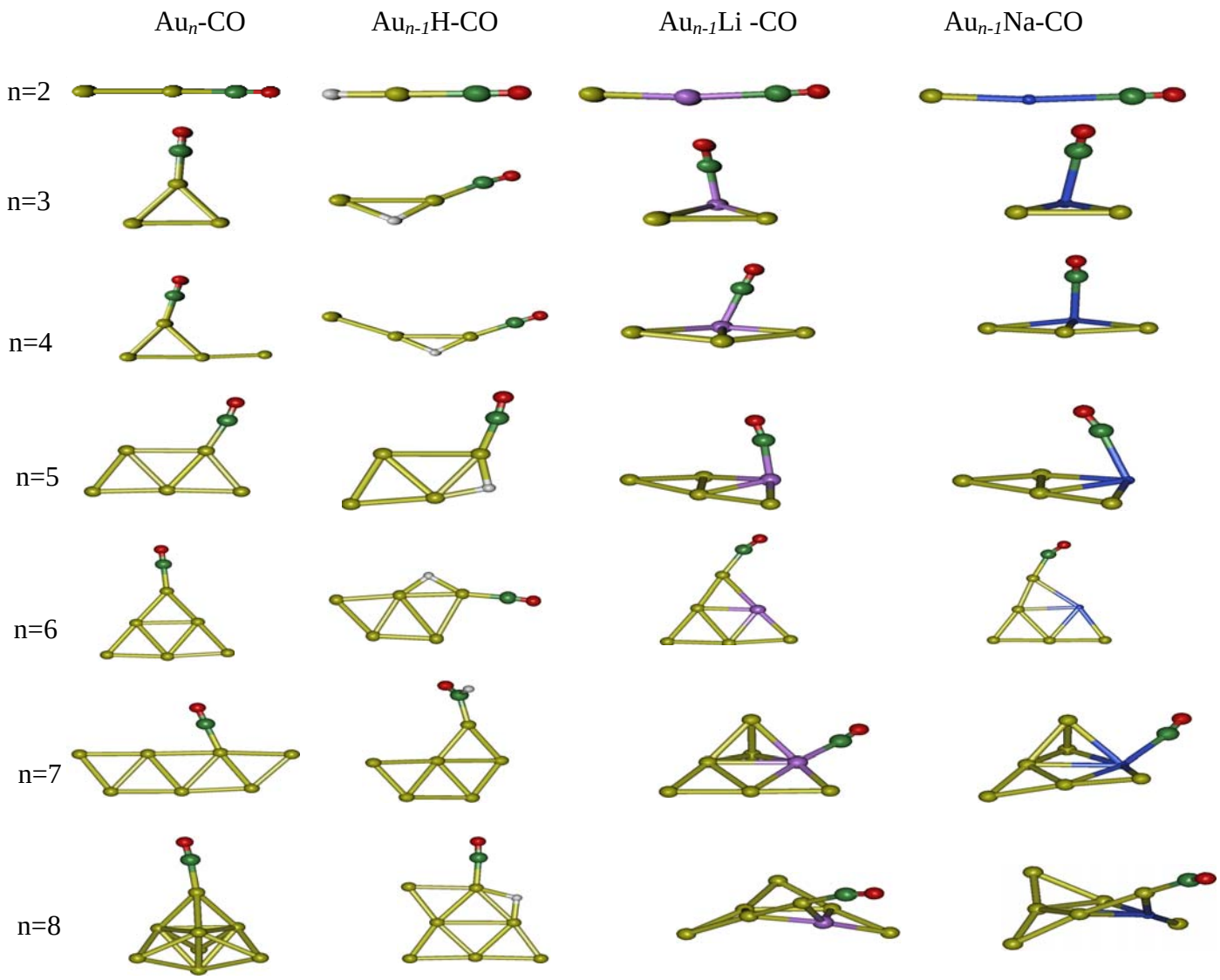

Figure SI-2