Electronic Supplementary Information (ESI)

Adsorption properties of pyramidal superatomic molecules based on the structure framework of Au_{20} cluster

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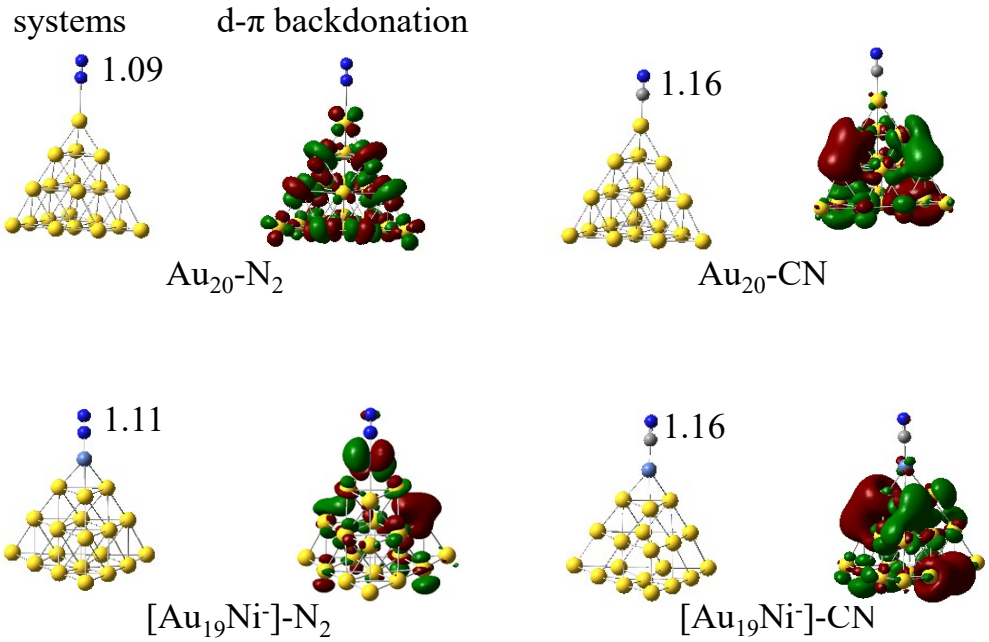

Fig. S1 The structures, bond lengths (Å) and the molecular orbitals of Au_{20}-N_2, [Au_{19}Ni-]-N_2, Au_{20}-CN, and [Au_{19}Ni-]-CN.

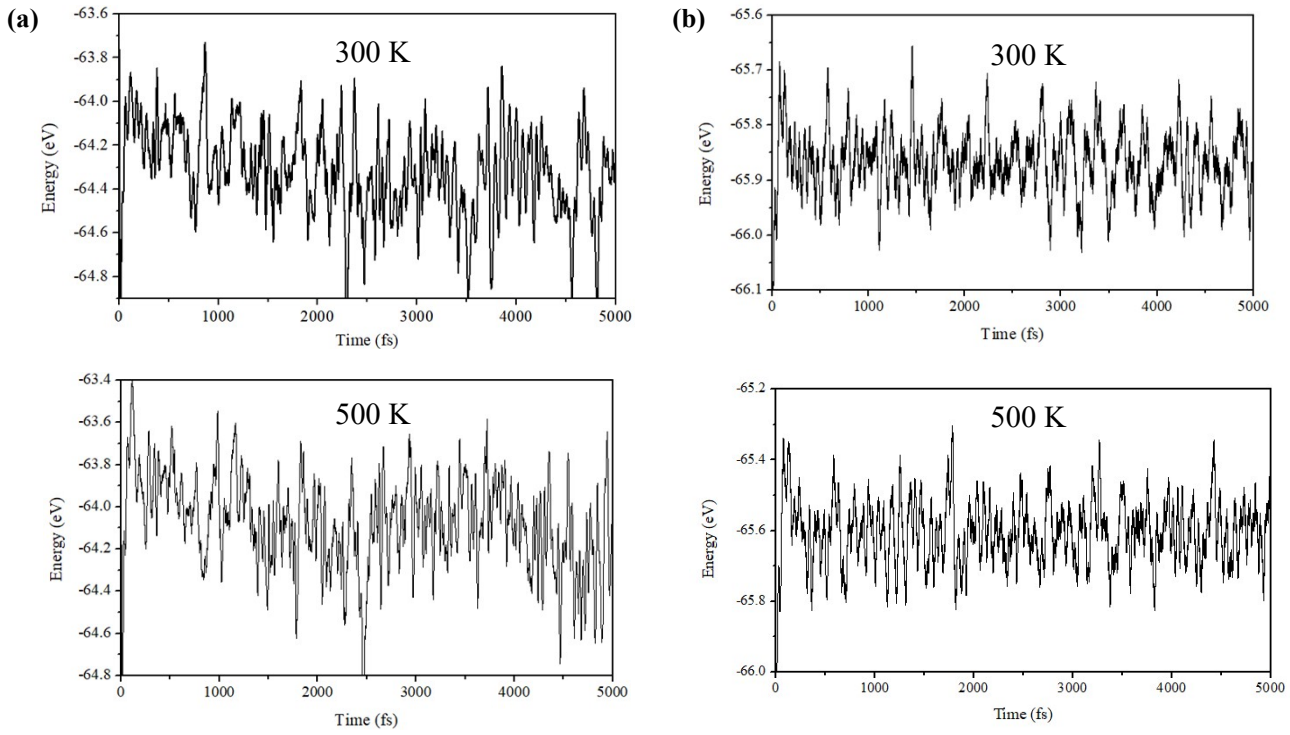

Fig. S2 Snapshots of the final frame of (a) $Au_{19}H$-CO and (b) Au_{20}-CO at the temperatures of 300 K and 500 K at the end of 10 ps AIMD simulations.

Table S1 NPA charge on the Au/Ni sites and the total charge on the adsorbed CO.

Systems	Charge on adsorption sites		ΔQ	Charge on CO after adsorption
	Before CO adsorption	After CO adsorption		
Au_{20}	0.18	0.16	-0.02	0.13
$Au_{19}Ni^-$	0.04	-0.17	-0.21	0.05