Supporting Information

Carbon Monoxide Adsorption on the Single-Walled Carbon Nanotube Supported Gold-Silver Nanoalloys

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Table 1. The QSC potential parameters for the different interactions

Interaction	ε (ev)	σ (Å)	n	m	C
Ag-Ag	0.0039450	4.0691	11	6	96.524
Au-Au	0.0078052	4.0651	11	8	53.581
Au-Ag	0.0055490	4.0671	11	7	75.0525

Table 2. The LJ potential parameters for the different interactions

Interaction	ε (ev)	σ (Å)
Ag - C (CNT)	0.030100	3.0650
Au - C (CNT)	0.034070	3.0030
Ag - C (CO)	0.039610	3.0370
Au - C (CO)	0.044830	3.0335
C (CO) - C (CO)	0.004553	3.4300
O (CO) - O (CO)	0.002601	3.1200
C (CO) - O (CO)	0.003441	3.2750
C (CO) - C (CNT)	0.003460	3.3995
O (CO) - C (CNT)	0.002615	3.2445
Au - O (CO)	0.033886	2.8785
Ag - O (CO)	0.029940	2.8820

Table 3. The details of the carbon nanotubes used in our simulations.

nanotube (n, m)	CNT diameter (nm)
(20, 0)	1.5
(26, 0)	2.0
(32, 0)	2.5
(38, 0)	3.0
(45, 0)	3.5
(11, 11)	1.5
(15, 15)	2.0
(19, 19)	2.5
(22, 22)	3.0
(26, 26)	3.5

We have also presented the snapshots of the CO adsorption and also the structure changes of the Ag-Au_{256} nanoalloy with the x_{Au}= 0.5 supported on the (18,0) CNT at 300 K in the supporting information (Figure S1). The left panel shows the adsorption of the CO molecules on the supported nanocluster. The right panel (up) shows the nanocluster before the inserting pressure (in vacuum) and the panel down shows the structure of the nanocluster after inserting the pressure by the gas.

Figure S1