Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Origin of Structural Stability of Cage-Like Au_{144} Clusters

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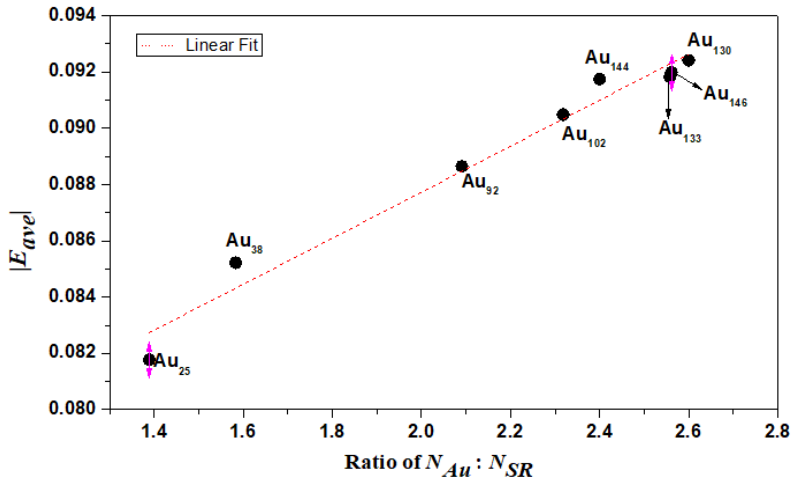

Figure S1. The averaged formation energy of $Au_{25}(SR)_{18}$, $Au_{38}(SR)_{24}$, $Au_{92}(SR)_{40}$, $Au_{102}(SR)_{44}$, $Au_{130}(SR)_{50}$, $Au_{133}(SR)_{52}$, $Au_{144}(SR)_{60}$, and $Au_{146}(SR)_{57}$ clusters, R is simplified by CH_3. The energy is in unit of Hartree.

Table S1. The BE and CE values and their ratios of two pairs of gold clusters.

	$Au_{145}(SCH_3)_{60}$	$Au_{144}(SCH_3)_{60}$	$Au_{133}(SCH_3)_{52}$	$Au_{132}(SCH_3)_{52}$
Shell-to-Core BE (eV)	-0.098	-0.098	-0.102	-0.101
Core CE (eV)	-0.094	-0.094	-0.094	-0.094
BE/CE	1.043	1.043	1.085	1.074

Table S1. Averaged formation energies of hollow/solid structures of sixteen gold clusters.

Au clusters	E_{ave} (Ha.)	Au clusters	E_{ave} (Ha.)
$Au_{145}(SCH_3)_{60}$	0.09185675	$Au_{142}(SCH_3)_{58}$	0.09097249
$Au_{144}(SCH_3)_{60}$	0.09199619	$Au_{141}(SCH_3)_{58}$	0.09096591
Au_{138} $(SCH_3)_{56}$	0.09110457	$Au_{136}(SCH_3)_{54}$	0.09126064
$Au_{139}(SCH_3)_{56}$	0.09110086	$Au_{135}(SCH_3)_{54}$	0.09128319
$Au_{133}(SCH_3)_{52}$	0.09219599	$Au_{130}(SCH_3)_{50}$	0.09263300
$Au_{132}(SCH_3)_{52}$	0.09212413	$Au_{129}(SCH_3)_{50}$	0.09249509
$Au_{145}(CCH)_{60}$	0.10871870	$Au_{278}(SH)_{84}$	0.11970632

$Au_{144}(CCH)_{60}$	0.10872967	$Au_{279}(SH)_{84}$	0.11985410