Supporting Information For:
Behavior of “Free-Standing” Hollow Au Nanocages at Finite Temperatures: A BOMD Study

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Supp-Tab. 1: Distribution of Loewdin Atomic Charges in the Hexagonal Base of Au₁₈, Au₁₈-SPH Clusters.

Atom in Base	Atomic Charge	
	Au ₁₈	Au ₁₈ -SPH
Au(1)	0.0750	-0.0711
Au(2)	0.0899	0.0545
Au(3)	0.0746	0.0531
Au(4)	0.0744	0.0346
Au(5)	0.0899	0.0601
Au(6)	0.0748	0.0341
Au(Central)	-0.2634	-0.0976