SUPPORTING INFORMATION

Shape stability of truncated octahedral fcc metal nanocrystals

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Figure S1 shows formation of 2D islands on a {111} side facet of truncated octahedra for "moderate" $N \approx 1.5\times10^4$ atoms for truncations TR2-TR4 and for somewhat higher T than considered for small $N \approx 0.8 \times 10^4$ in the main text. Features to note are: (i) edges of the NC are now active with atoms being removed and populating {100} and {111} facets; (ii) mass transport now occurs between {100} facets leading to the formation of 2D near-square islands on top of those {100} facets; (iii) single atoms and smaller clusters on {111} facets are common in addition to the larger cluster with the $q^* = 19$ atom hexagonal core. We also comment on these features in the Discussion section.

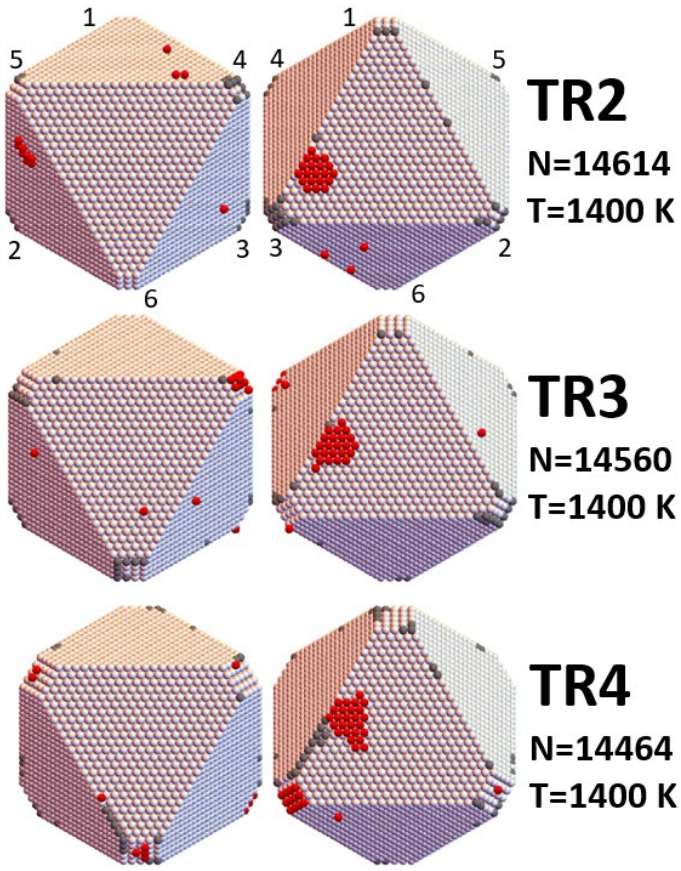

Figure S1. KMC simulation images showing the formation of this first island on a {111} facet including a q*=16 hexagonal core. Two images from different perspectives are shown for each NC (vertex labeling as shown for TR1 helps to relate these). Shown are NCs for "medium" $N \approx 1.5\times10^4$ atoms for truncations TR2-TR4 and for T = 1400 K. Grey: initially populated sites, now empty. Red: initially empty sites now populated.