Electronic Supplementary Material (ESI) for Nanoscale.

On-surface synthesis of size- and shape-controlled two-dimensional Au_n nanoclusters using a flexible fullerene molecular template

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Figure S1 shows three STM images acquired one after another from the same area of the sample at room temperature. In the left panel, we see seven large bright spots. These large spots are Au clusters floating on top of the C_{60} monolayer. One of the floating clusters is highlighted with a circle. In the middle panel, it can be seen that the highlighted cluster is moved by the STM tip. A small fraction, the bottom ¼, of the cluster is imaged at its initial location. Then it moves all of a sudden to the left as indicated by the arrow. In the right panel, the moved cluster is observed at its new location, although it is moving. At the location initially occupied by this cluster, we see close-packed C_{60} molecules. These STM images demonstrate that the large bright spots are Au clusters sitting on top of the C_{60} layer. These clusters are weakly attached to the C_{60} layer and can be moved by the STM tip under normal scanning conditions at RT.

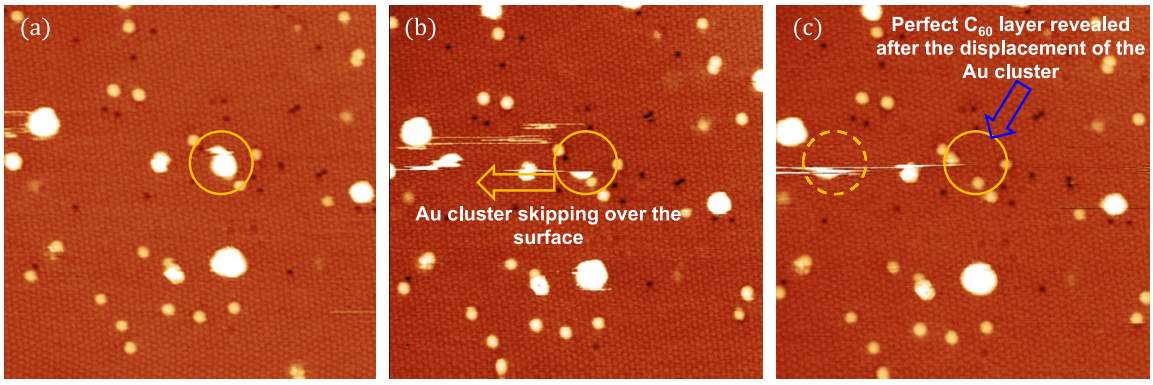

Fig. S1 Successive STM images showing the movement of a floating Au cluster. Image size: 55 nm x 55 nm. Image parameters: +1.7 V; 50 pA.

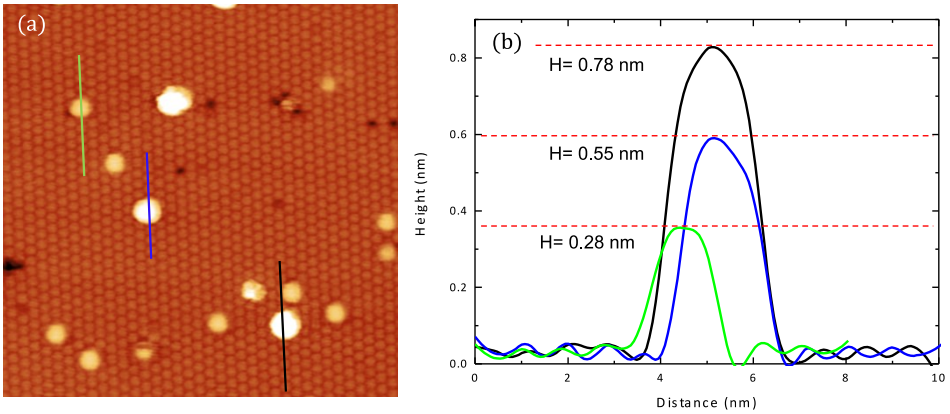

Fig. S2 (a) STM image obtained with +1.7 V sample bias and 50 pA tunnel current. (b) Height profiles along the green, blue, and black lines in (a), respectively. Height profile along the green line in (a) shows that the corresponding bright C_{60} is ~ 0.28 nm tall. The height profiles along the blue line and the black line are for two floating Au clusters.

Figure S2(a) shows two types of bright spots: Single raised C_{60} molecules and larger brighter features due to the floating Au clusters. The height profiles for three bright spots are displayed in (b). Figure S3 is a histogram plot of the height distribution of single raised C_{60} molecules in the first molecular layer. The sample has been annealed to 425 K. There are clearly two peaks. The peak at ~0.28 nm shows that the majority of the raised C_{60} molecules sit on single-atomic-layer Au islands. The peak at ~0.63 nm shows that a small fraction of the C_{60} molecules sit on double-atomic-layer Au islands.

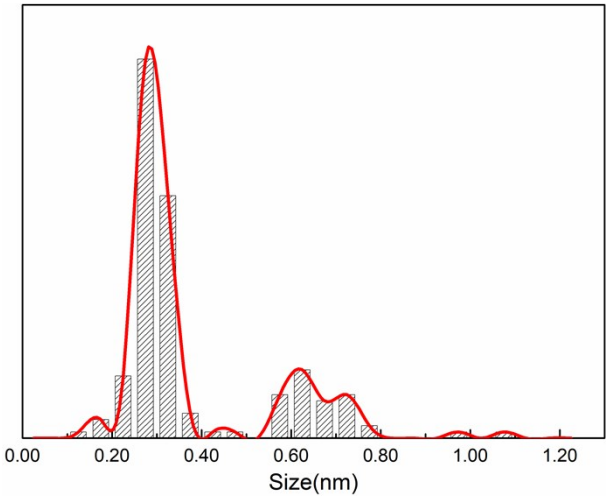

Fig. S3. Histogram of cluster height distribution. This plot is based on measurement from a sample that has been annealed to 425 K. The height distribution has two peaks: one at~ 0.28 nm due to C_{60} molecules sitting on a single layer of Au atoms; and the other at ~0.63 nm which is due to C_{60} molecule sitting on two layers of Au.

The structural stability of Au(x=19) cluster is further checked by MD calculations at 300 K. In MD calculations, bigger supercells and four layers of substrate are considered (Figs. S4a and 4b). Figure S4c plots the center-of-mass coordinates of an Au(x=19) cluster as a function of the simulation time. For the annealing process, the system is heated from 100 K to 375 K over 275 ps. The system is then maintained at 375 K and simulation is performed for 20 ns. Finally the system is cooled down from 375 K to 300 K over 75 ps

and simulation is performed at 300 K for 20 ns. The center-of-mass position does not change with time and is subject only to very small fluctuations. This demonstrates that the Au_{19} cluster is stable at RT.

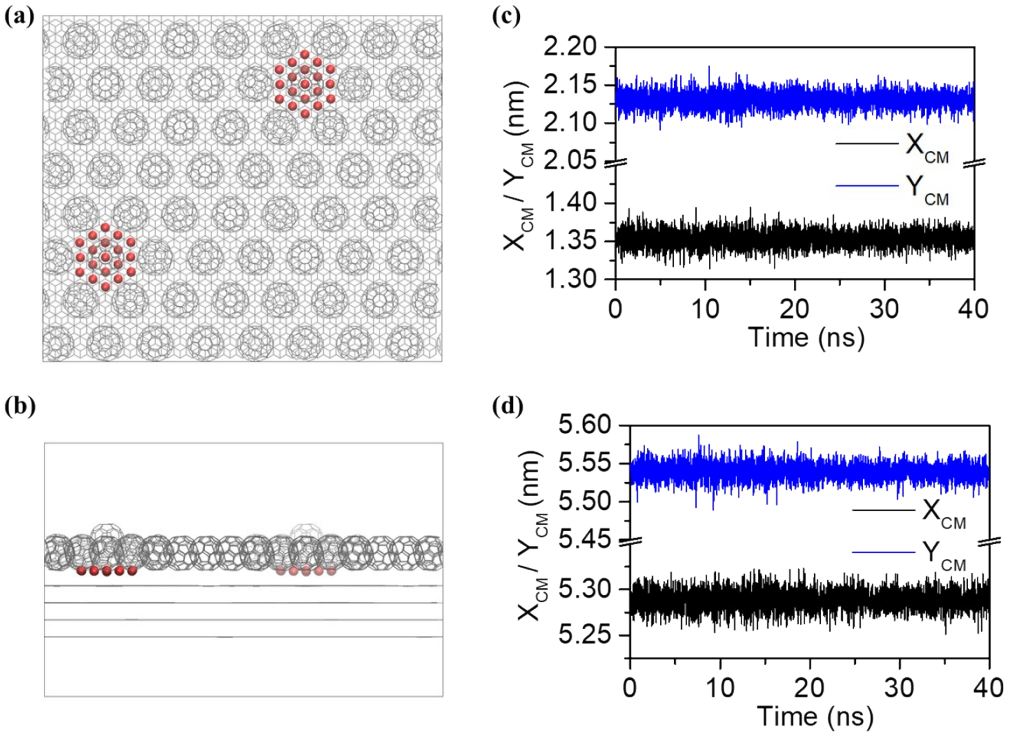

Figure S4. Molecular-dynamics simulation results at 300 K. (a) Top view and (b) side view of the atomic model in the MD calculations. (c, d) The evolution of the center-of-mass position as a function of the simulation time for the lower left and the upper right Au_{19} clusters in (a), respectively. X_{CM} and Y_{CM} are the (x,y) coordinates of the center of mass of the cluster.

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