Supporting information for

The effects of 1-pentyne hydrogenation on the atomic structures of size-selected \( \text{Au}_N \) and \( \text{Pd}_N \) (\( N=923 \) and 2057) nanoclusters

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S0.1 Atomic structures of \( \text{Au}_{2057} \) following thermal treatment

Fig. S1 shows the proportions of isomers of \( \text{Au}_{2057} \) nanoclusters both before and after thermal treatment.

\[ \text{Au}_{2057} \]

**Figure S1.** Charts showing the proportions of \( \text{Au}_{2057} \) isomers (a) before thermal treatment, (b) after storage in vacuum at RT, (c) after thermal treatment under a gas flow of pure He (279 ml/min), and (d) after thermal treatment under a gas flow of 40% \( \text{H}_2 \) + 60% He (247 ml/min). Thermal treatment was conducted at 523 K for 2 hours (ramp rate of 2°C/min from RT). Related cluster formation parameters: condensation length, 250 mm; magnetron sputtering power, 10 W DC; condensation pressure, 0.67 mbar; deposition energy, 0.5 eV/atom; condensation gas flows, rate 200 sccm (Ar) and 150 sccm (He).
S0.2 Stability of nanocluster structure under the electron beam

Fig. S2 shows a series of images, taken consecutively, revealing the atomic structure (in this case, face-centred cubic) of a size-selected Au$_{923}$ nanocluster. Each image is captured over a period of 5.49 s. Although the nanoclusters may rotate slightly from one image to the next, the nanocluster remains as face-centred cubic throughout. Hence, this demonstrates that the nanocluster structure maintains its integrity under the electron beam.

**Figure S2** A series of HAADF-STEM images, taken consecutively, of a size-selected Au$_{923}$ nanocluster exhibiting a face-centred cubic (fcc) structure. Each image is captured over a period of 5.49 s.