

Supplementary Materials for

Energy Landscape of Au₁₃: A global view of structure transformation

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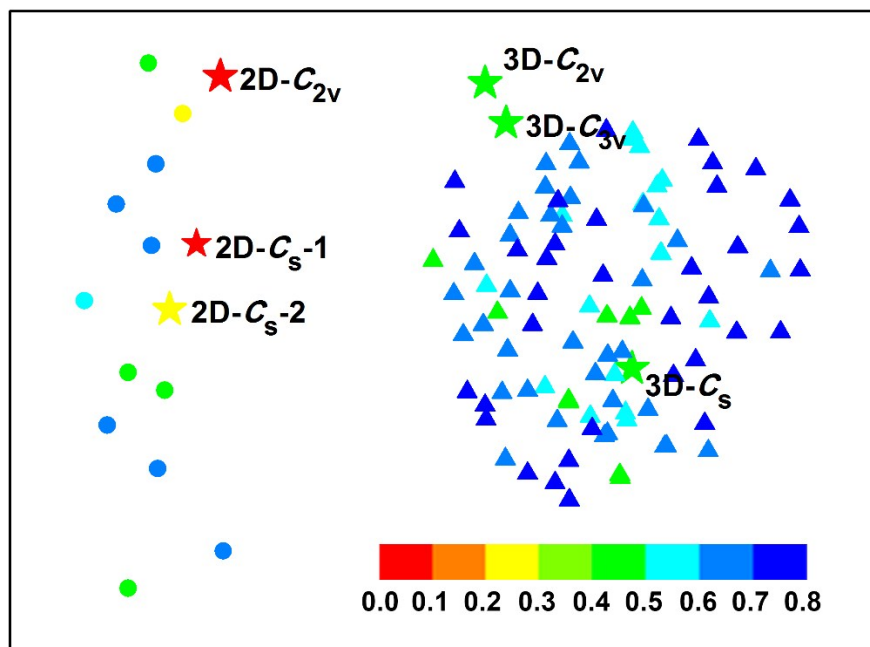


Fig. S1 2D landscape of Au_{13} cluster. Each point here represents a local minimum configuration, whose position on the 2D map is determined by minimizing $\sum_{p < q} (d_{2D,pq} - d_{\text{dist},pq})^2$. The circular and triangular points represent 2D and 3D configurations respectively, while the stars represent the six lowlying configurations particularly, as referred in the maintext (see Fig. 2). The colors stand for the energies of the configurations, as indicated by the color bar.

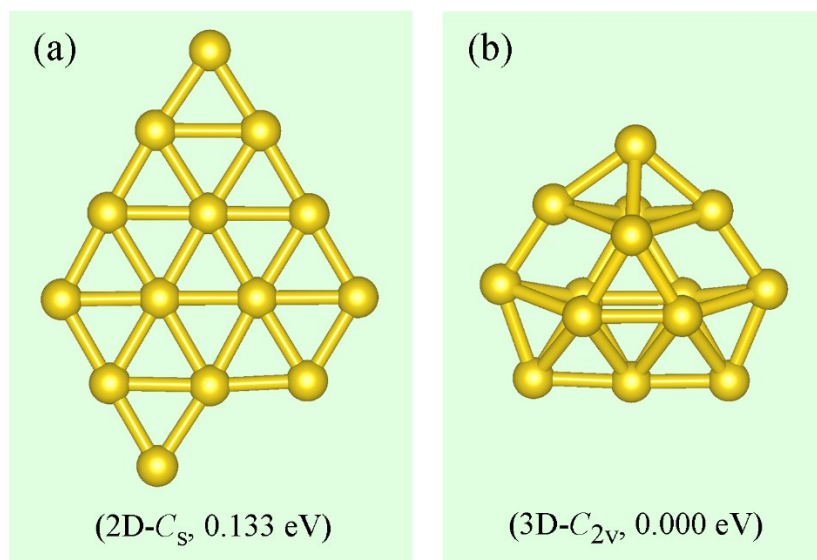


Fig. S2 Low energy configurations of Au_{14} with (a) two-dimensional (2D) structure and (b) 3D structure. The energies are with respect to the global minimum 3D- C_{2v} .

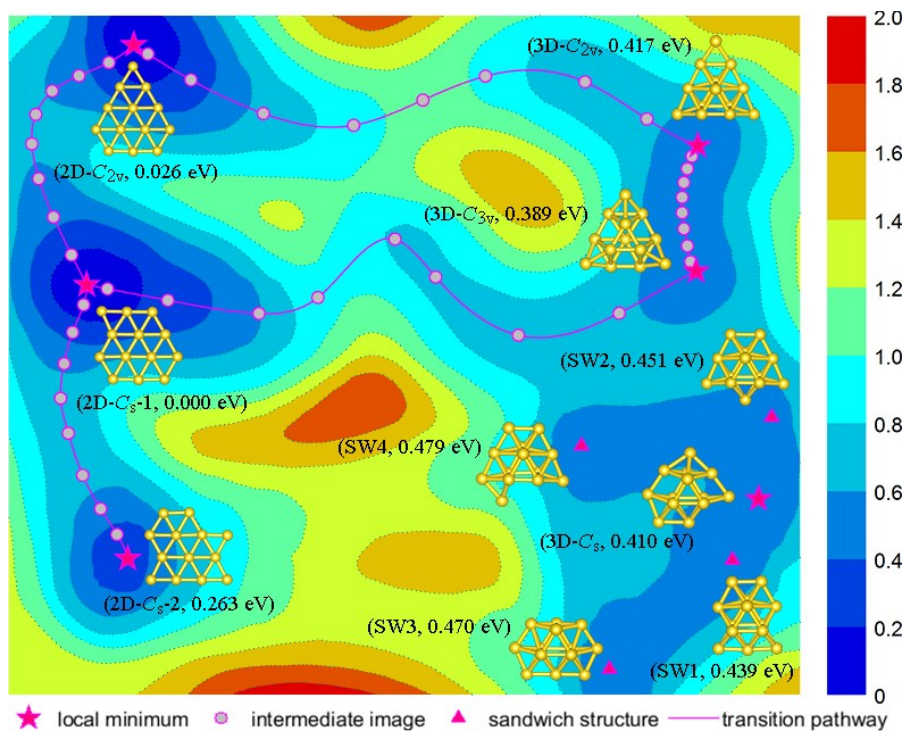


Fig. S3 Artificial 2D contour map showing the detailed landscape of Au_{13} around 3D-C_s . The triangles represent a series of sandwich (SW) configurations with different interlayer structures, whose surrounding landscape was obtained by the distance-barrier correlation and interpolation, while the rest of the map is sketched as Fig. 2. Obviously, 3D-C_s and the SW configurations have relatively similar structures and form a corrugated basin on the potential energy surface, leading to the flexuosity of pathways from other local minima towards 3D-C_s .

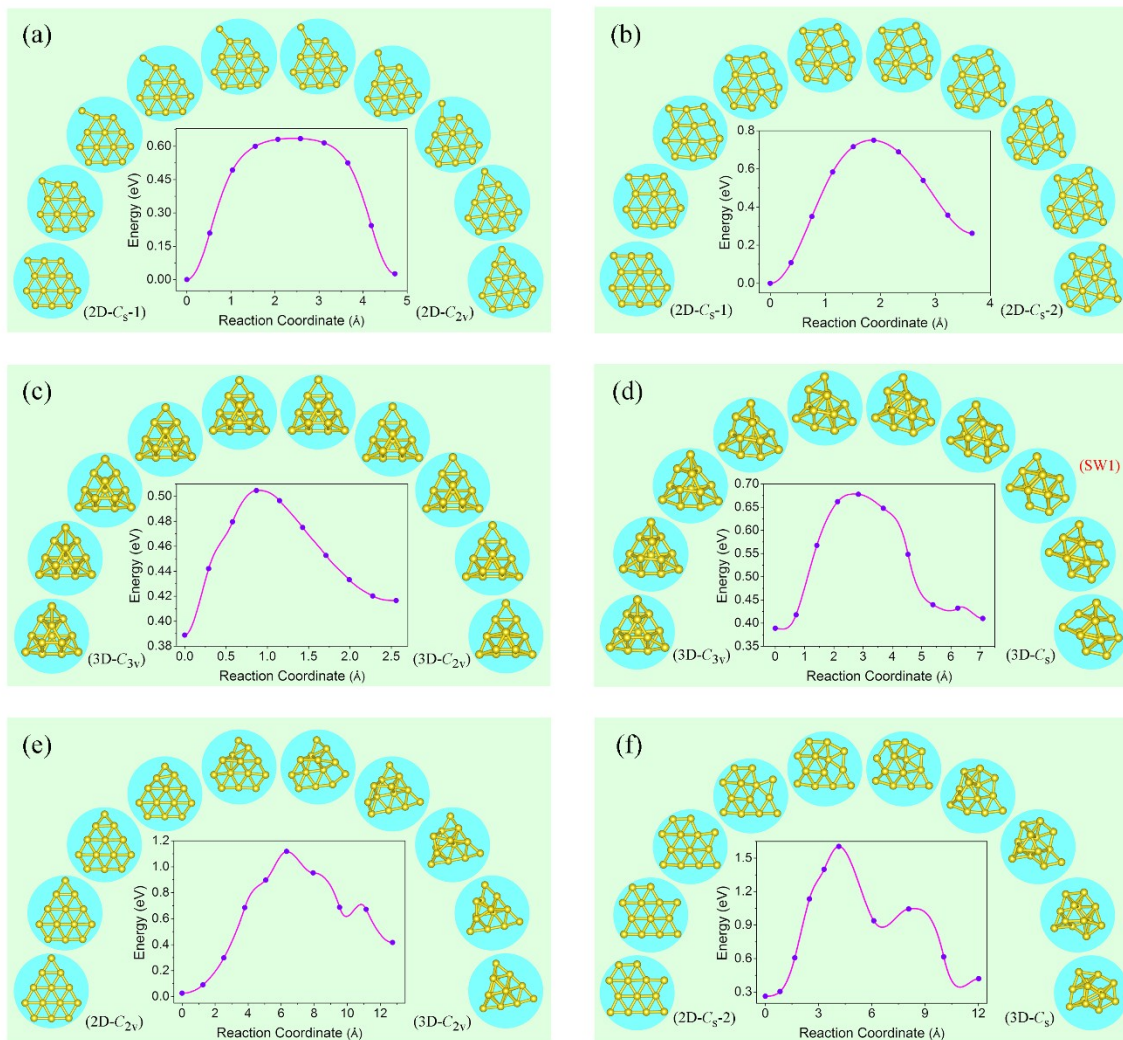


Fig. S4 Detailed pathways between the representative configurations in Fig. 2, with selected images in the transition. Note that the pathway between $3D-C_{3v}$ and $3D-C_s$ in (d) passes through SW1, leading to two irregular images alongside the path in Fig. 2 (refer to the position of SW1 on the PES in Fig. S3).