Electronic Supplementary Material (ESI) for Soft Matter.

Supporting information for:

Interaction between capped tetrahedral gold nanocrystals: dependence on effective softness

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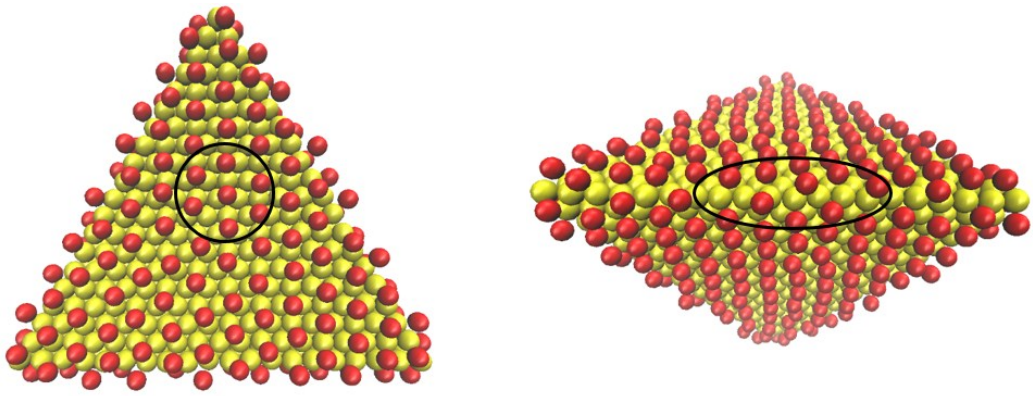

Figure S1. Snapshots of SH groups (a) in the center and (b) on the edge of (111) facet of an equilibrated 5.6 nm edge length SC_{16}-capped tetrahedral gold NC. Yellow and red spheres represent gold atoms and SH groups, respectively. In the centers of (111) facet the hexagonal arrangement is observed, while on the edges zigzag organization appears.

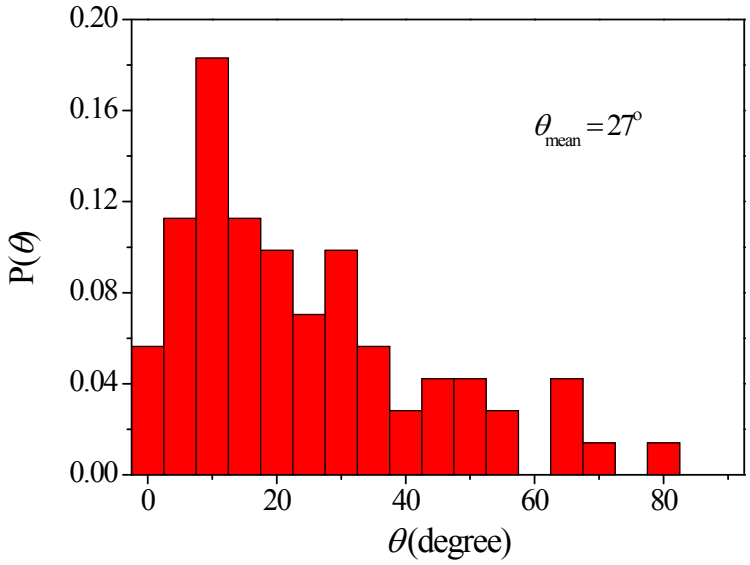

Figure S2. The distribution of angle θ for all ligands on the (111) facet of an isolated 5.6 nm SC_8-capped tetrahedral gold NC. The angle θ_i for the *i*-th ligand chain is defined as $\theta_i = \arccos(\vec{h}_i \cdot \vec{z} / |\vec{h}_i|)$, where the end-to-end vector $\vec{h}_i = \vec{r}_{i,\mathrm{CH_3}} - \vec{r}_{i,\mathrm{S}}$ and z is the unit vector perpendicular to the facet. Here $\vec{r}_{i,\mathrm{CH_3}}$ and $\vec{r}_{i,\mathrm{S}}$ represent the coordinates of the CH_3 and SH group, respectively. The calculated mean value θ_{mean} for all ligands is 27^0.

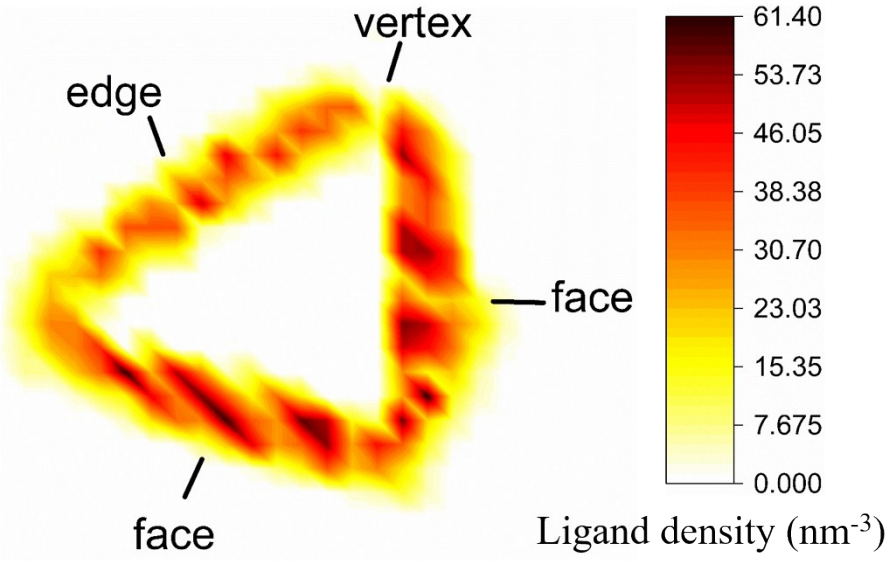

Figure S3. Two-dimensional plot of the ligand bead (SH, CH_2, and CH_3) density of SC_8 chains around the tetrahedral gold core of 5.6 nm edge length. The ligand density profile is viewed along the direction that is perpendicular to the symmetrical cross section passing through the center and an edge of the tetrahedral NC. The white triangle represents the position of the tetrahedral core. The color code indicated by the bar gives the average number of ligand beads per nm^3. The two-dimensional plot clearly shows that the passivated NC is geometrically anisotropic. It can be seen from the figure that the density of ligand molecules is the smallest on the vertex, the secondly on the edge, and the highest on the (111) facet, which is consistent with the snapshots in Figs. 5(a)-(c).

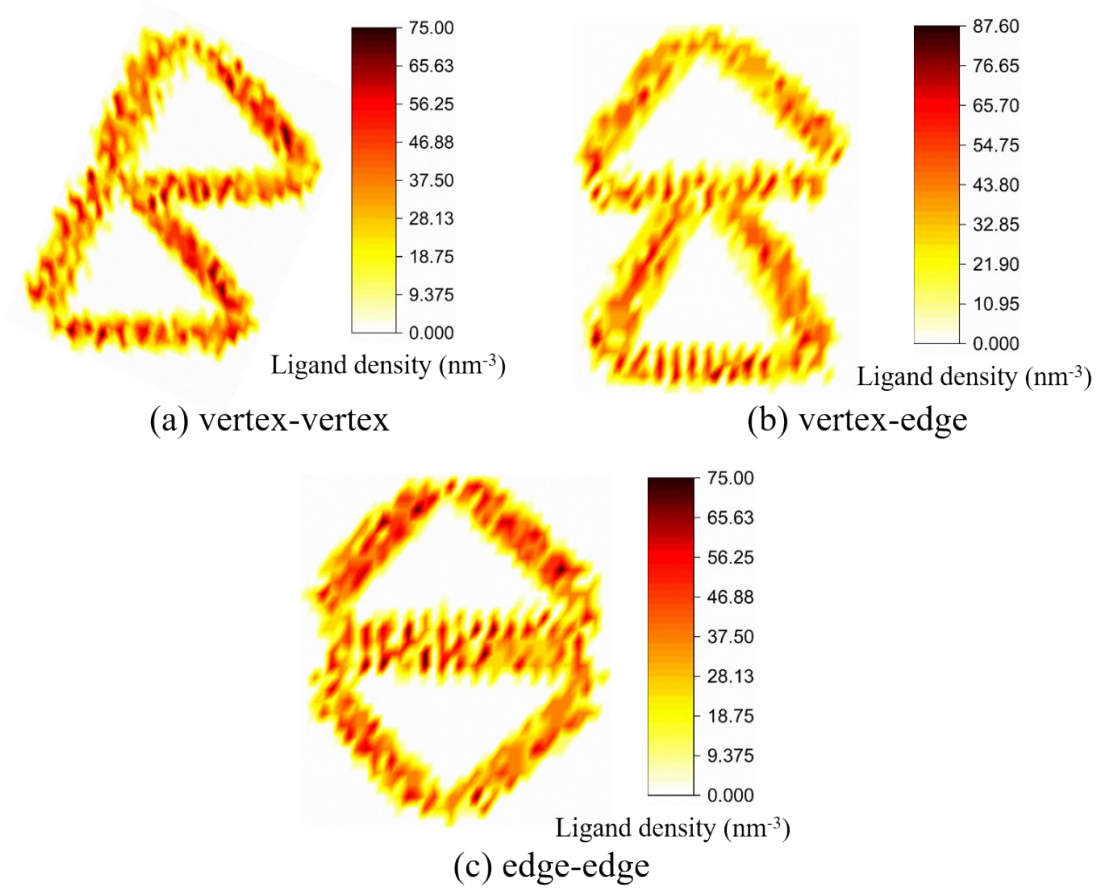

Figure S4. Density profiles of capping ligands for two equilibrated SC_8-capped tetrahedral gold NCs of 5.6 nm edge length in (a) vertex-vertex, (b) vertex-edge, and (c) edge-edge orientations. Systems are viewed along the direction that is perpendicular to the symmetrical cross section passing through the two centers of tetrahedral NCs. The profiles are colored with the same scheme as in Fig. S3, and the two white triangles in each case correspond to the NC cores. One can observe substantial interdigitation of ligand chains for all three cases, which is consistent with the scenarios in Fig. 6(a).

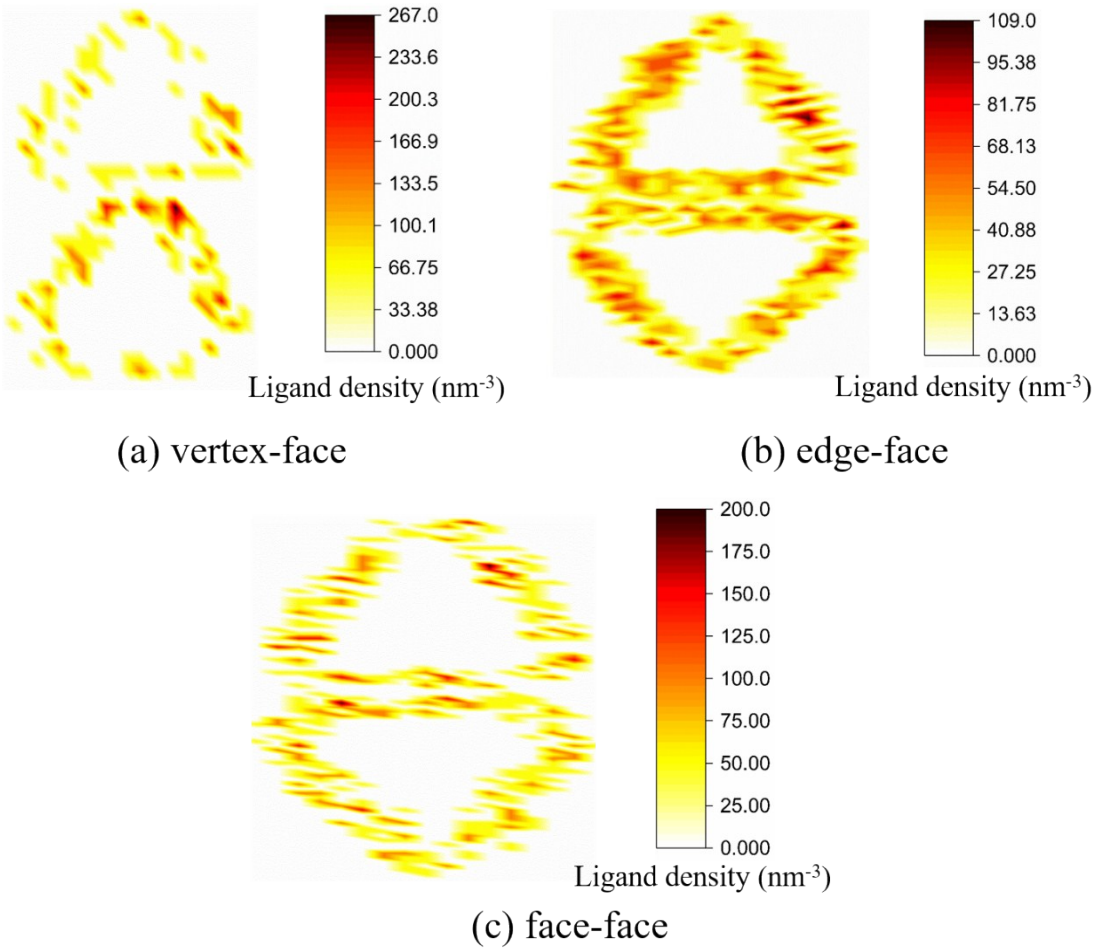

Figure S5. Density profiles of capping ligands for two equilibrated SC_8-capped tetrahedral gold NCs of 5.6 nm edge length in (a) vertex-face, (b) edge-face, and (c) face-face orientations. Systems are viewed along the direction that is perpendicular to the symmetrical cross section passing through the two center of tetrahedral NCs. The profiles are colored with the same scheme as in Fig. S3, and the two white triangles in each case correspond to the NC cores. In these three cases, obvious gaps are observed between the two capping layers of tetrahedral NCs. This means that there is little ligand interdigitation between two tetrahedral particles in vertex-face, edge-face, and face-face orientations, which is consistent with the snapshots in Fig. 6(b).