Electronic Supplementary Material (ESI) for RSC Advances.

Supplemental Materials

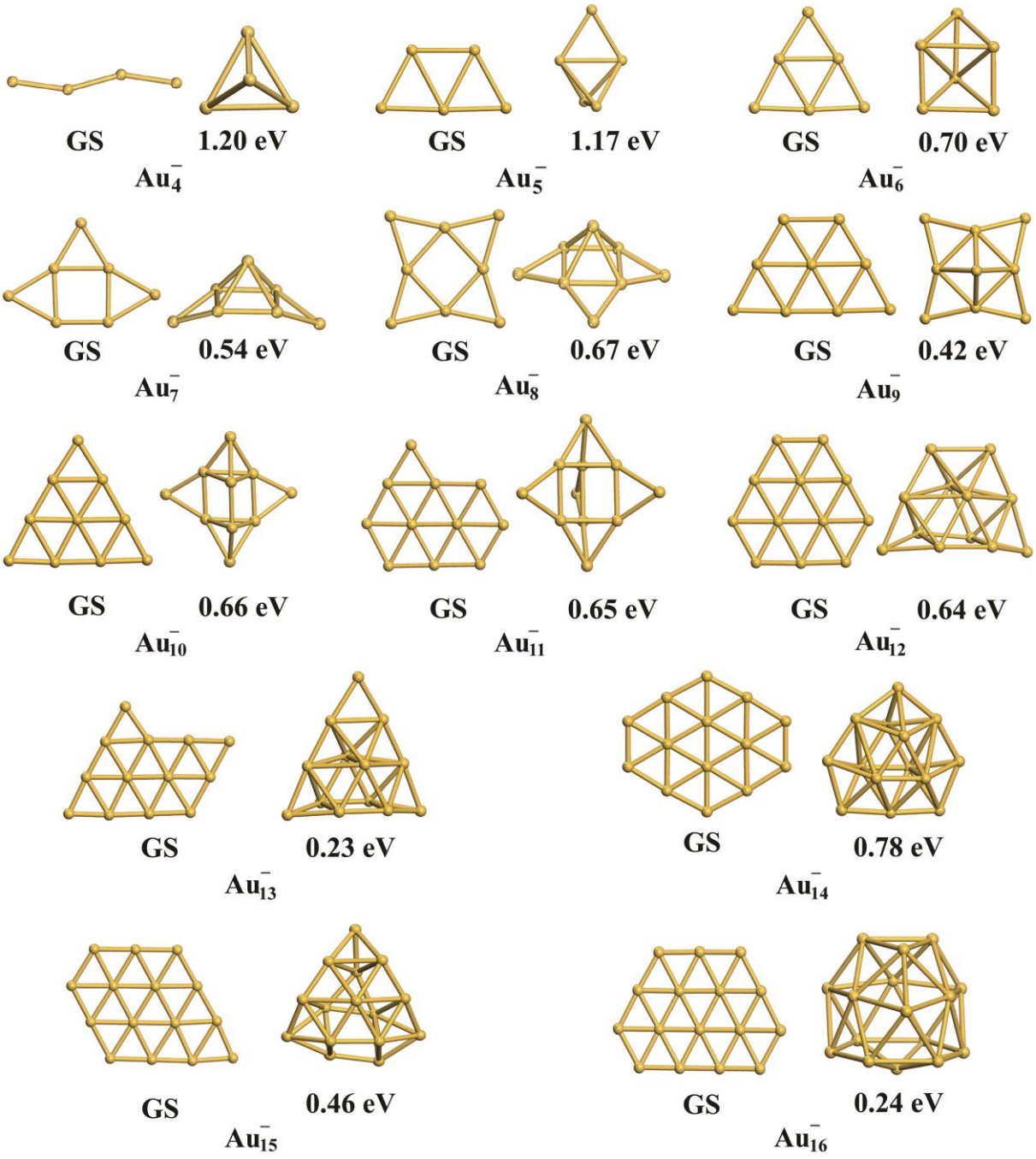


Figure S1 The lowest energy 2D and 3D structures among the corresponding planar and non-planar structures studied by using PBE functional for Au_n^- anionic clusters, respectively. The GS stands for the ground state structure. The relative energy is provided below the corresponding isomer.

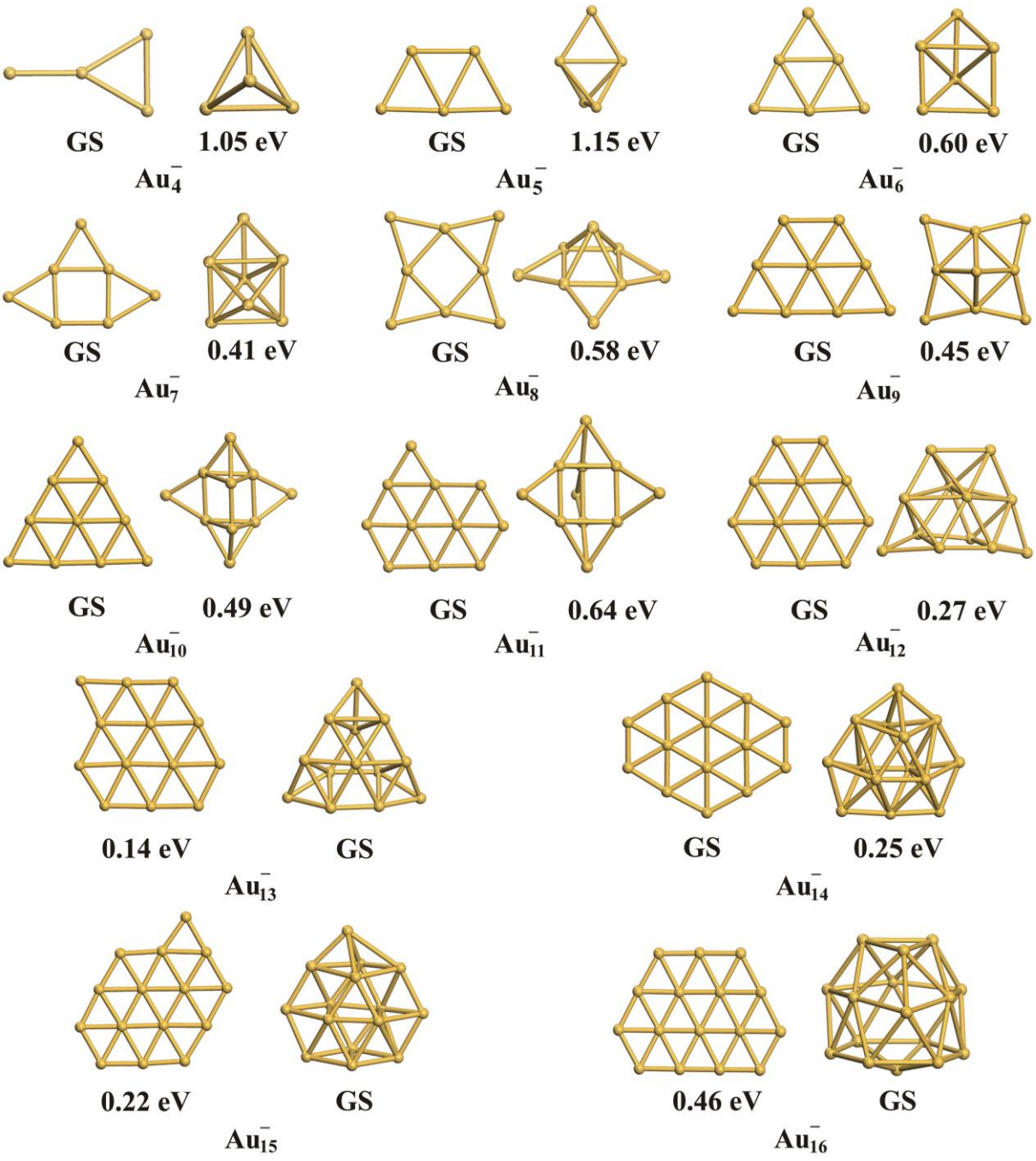


Figure S2 Same as the caption of Fig. S1 except that the above results are calculated by using PBEsol functional.

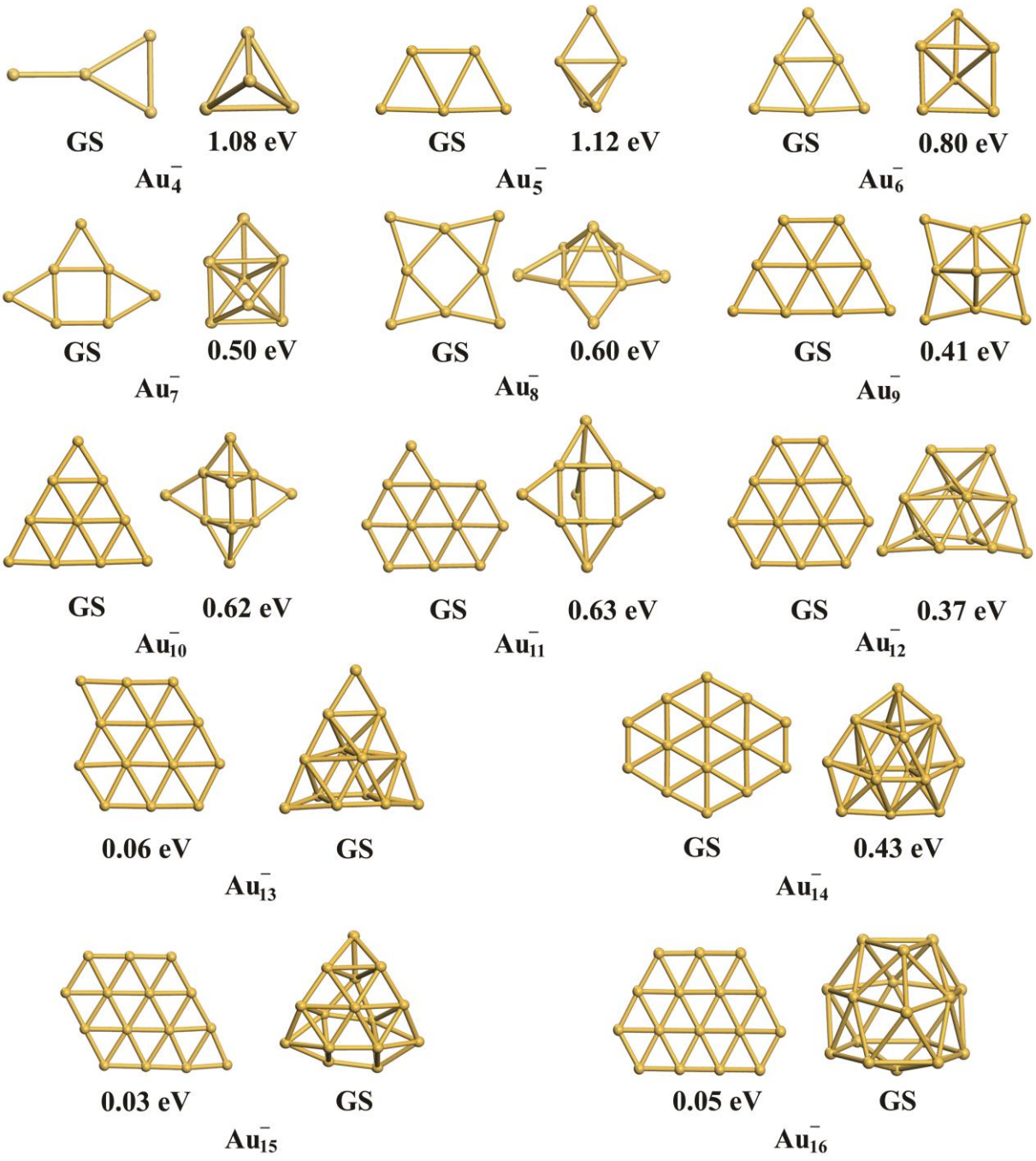


Figure S3 Same as the caption of Fig. S1 except that the above results are calculated by using meta-GGA TPSS functional.

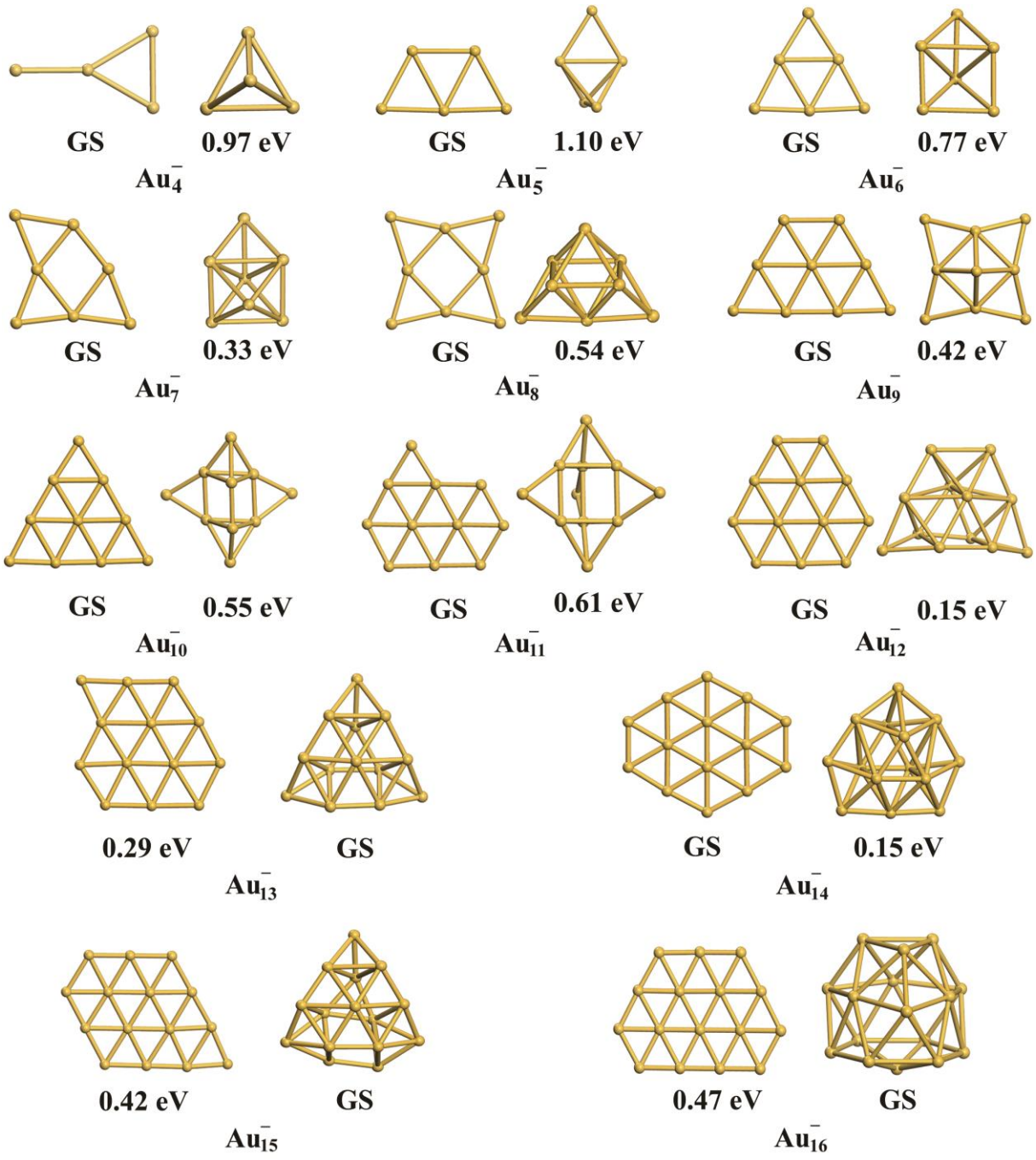


Figure S4 Same as the caption of Fig. S1 except that the above results are calculated by using meta-GGA revTPSS functional.

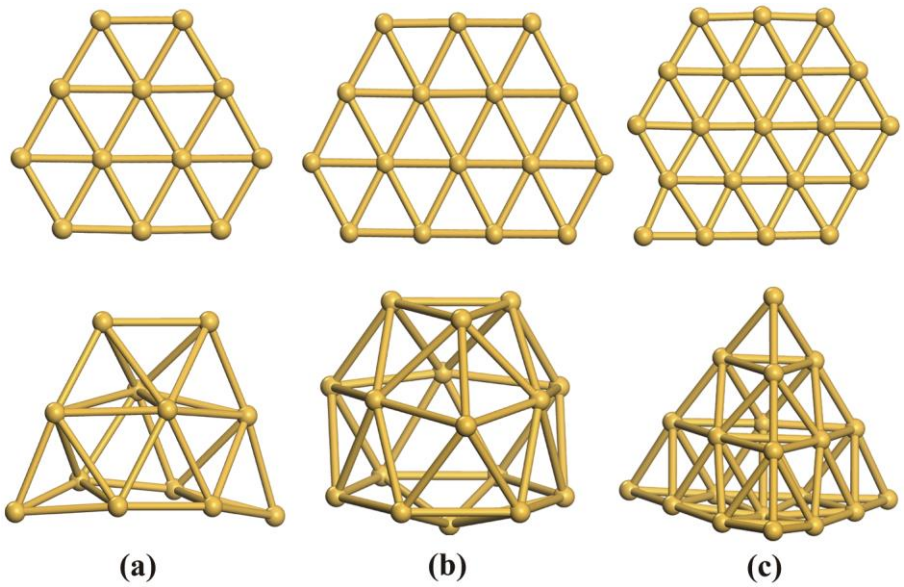


Figure S5 The lowest energy 2D and 3D structures among the corresponding planar and non-planar structures for Au_{12}^-, Au_{16}^-, and Au_{20}^- anionic clusters.

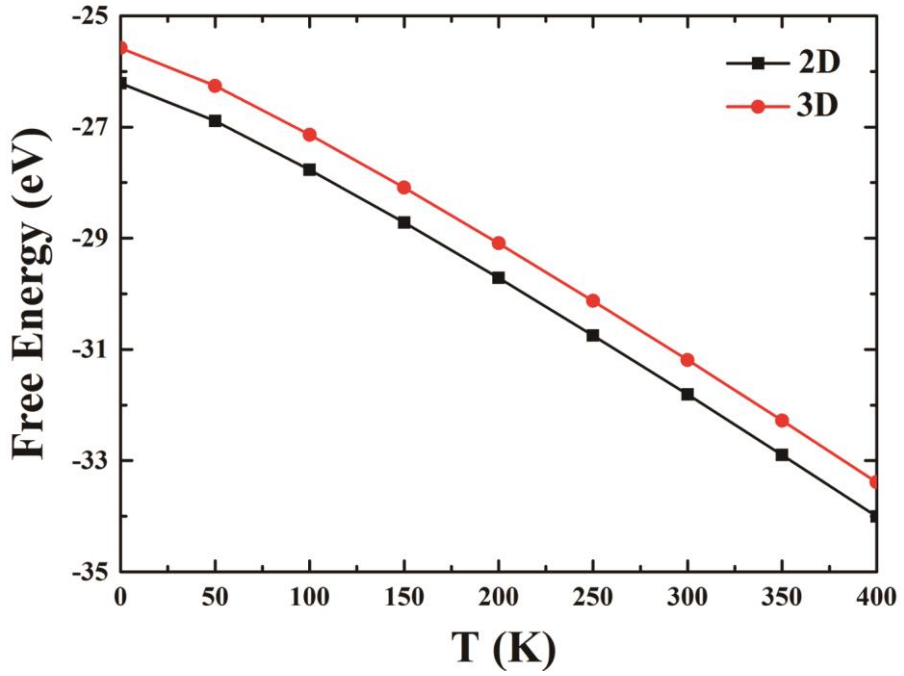


Figure S6 The evolution of the calculated free energy as a function of temperature for the selected 3D geometry as shown in Fig. 2 as well as the corresponding 2D structure for Au_{12}^- cluster.

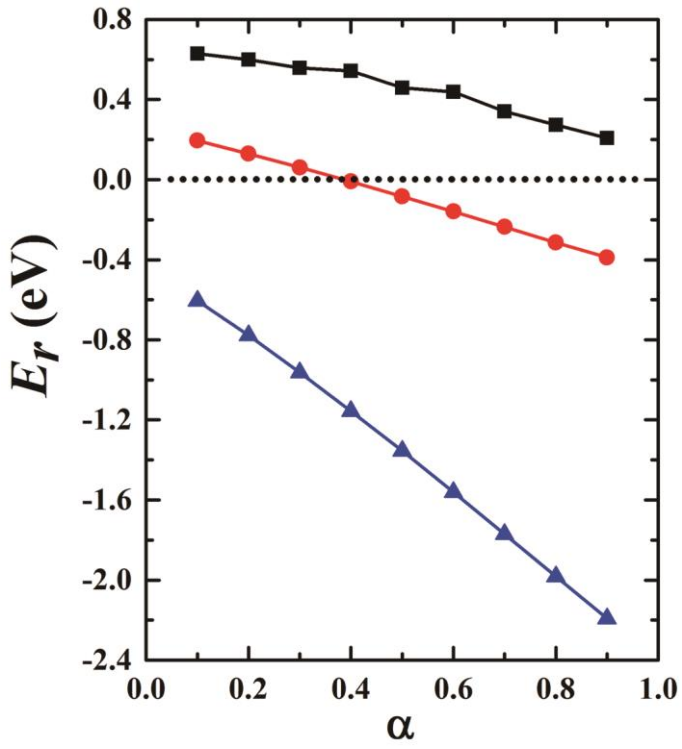


Figure S7 The relative energy calculated with HSE functional versus the hybridization ratio α of the 3D geometries as shown in Fig. 2 for the Au_{12}^-, Au_{16}^-, and Au_{20}^- anionic clusters as referred to the corresponding 2D structures.

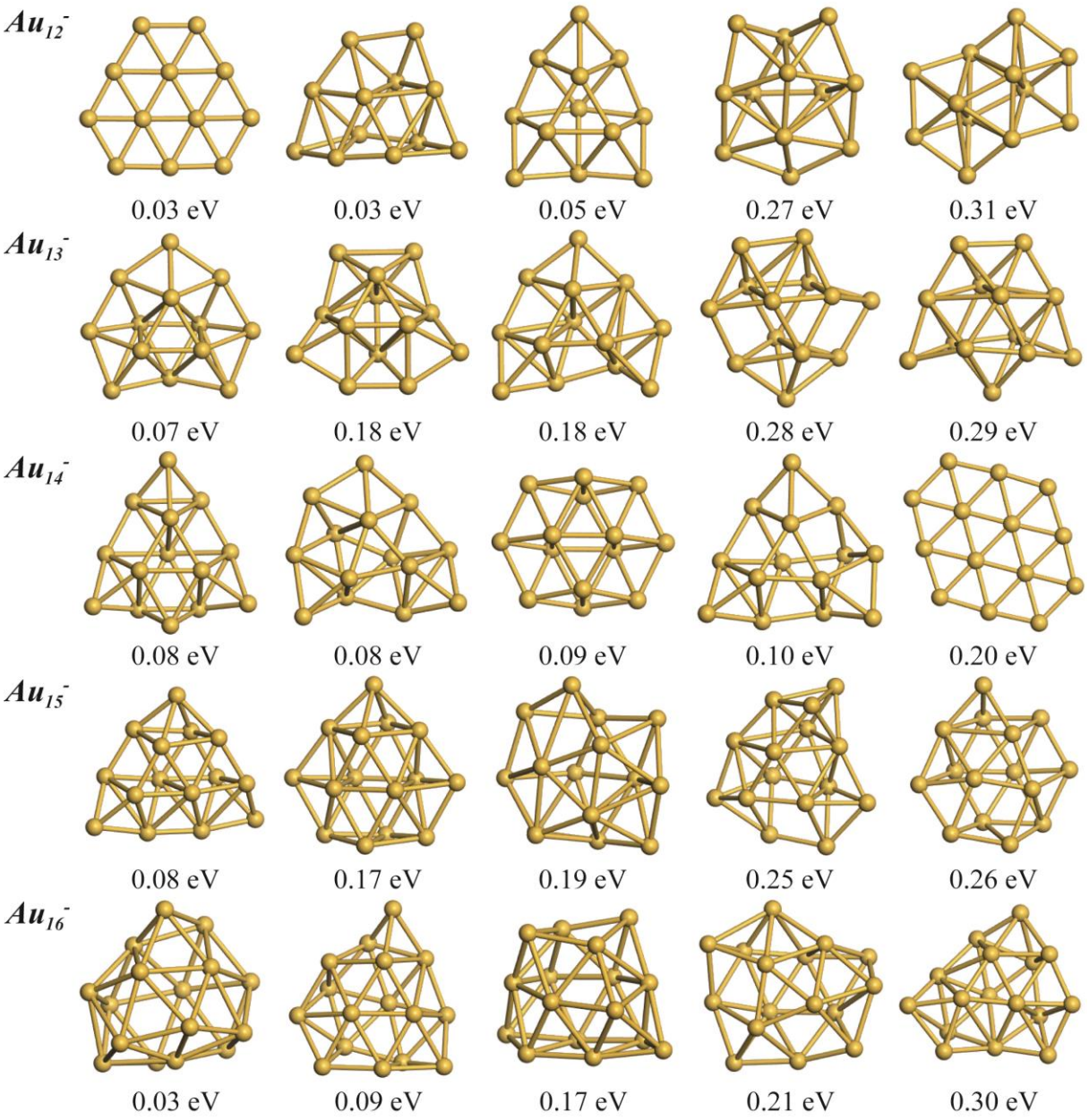


Figure S8 The first 5 low-lying isomers for the Au_n^- (n≥12) anions calculated by using the TSD-PBE method. The relative energy is provided below the corresponding isomer.

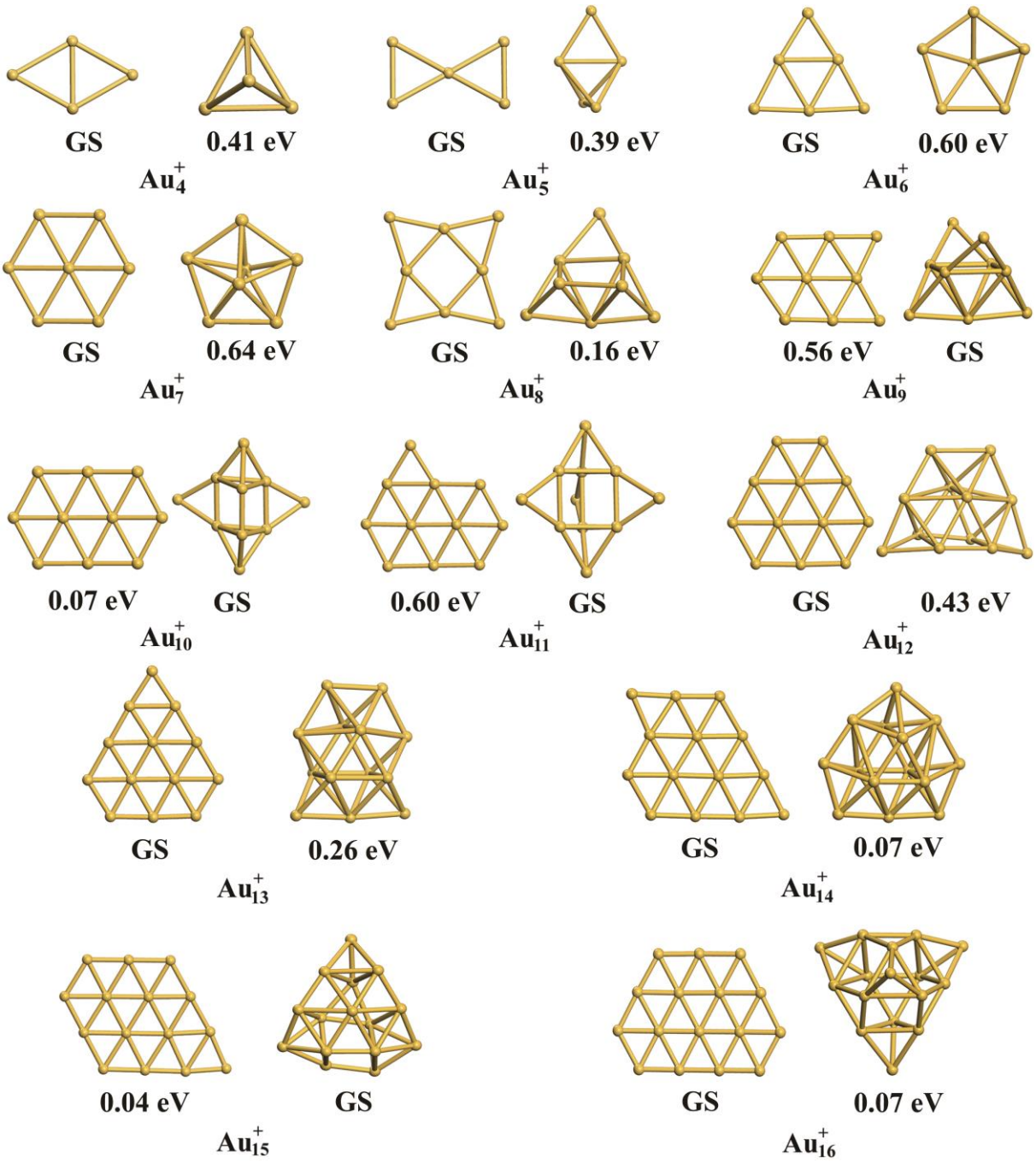


Figure S9 The lowest energy 2D and 3D structures among the corresponding planar and non-planar structures studied by using PBE functional for Au_n^+ cationic clusters, respectively. The GS stands for the ground state structure. The relative energy is provided below the corresponding isomer.

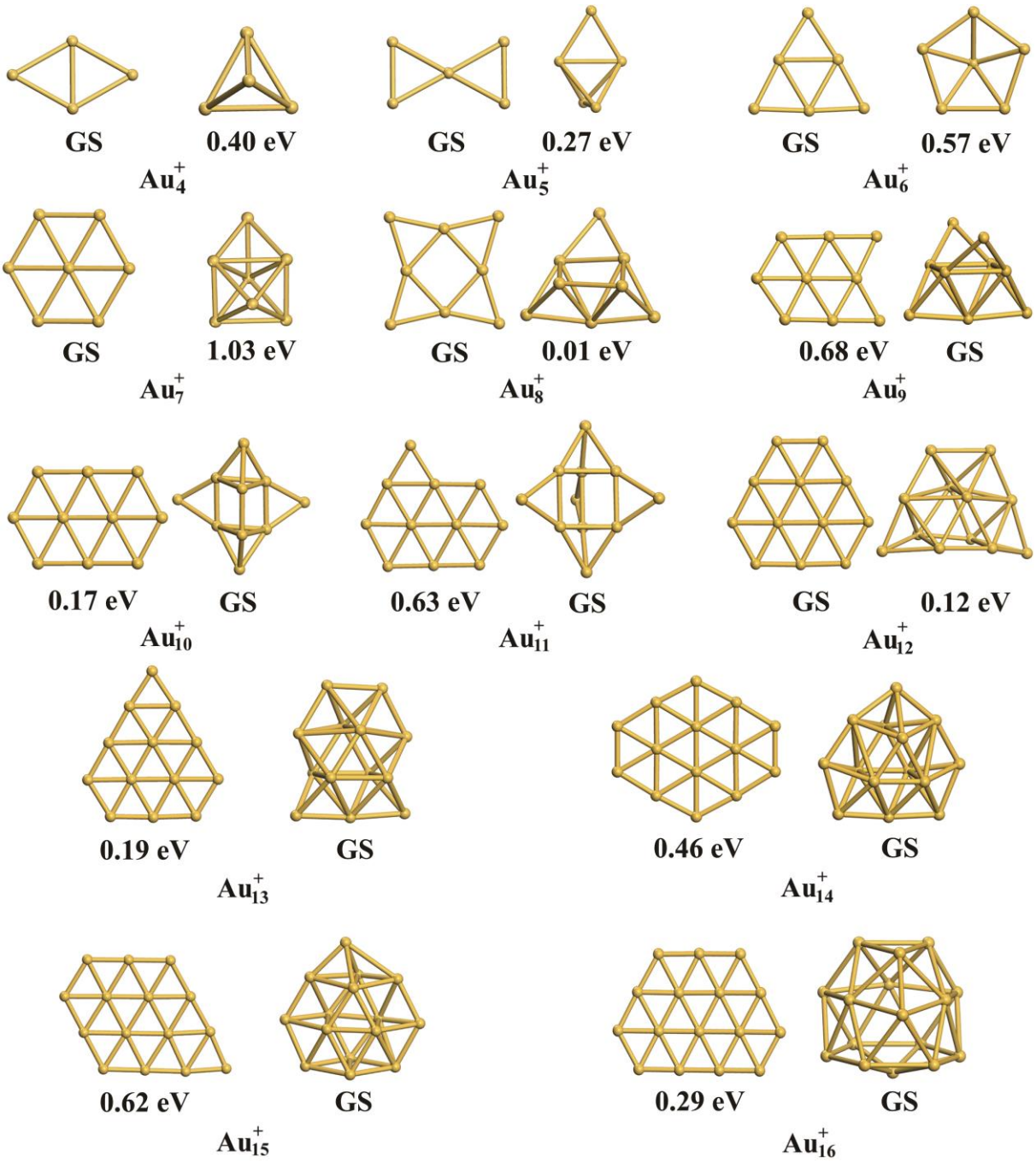


Figure S10 Same as the caption of Fig. S9 except that the above results are calculated by using PBEsol functional.

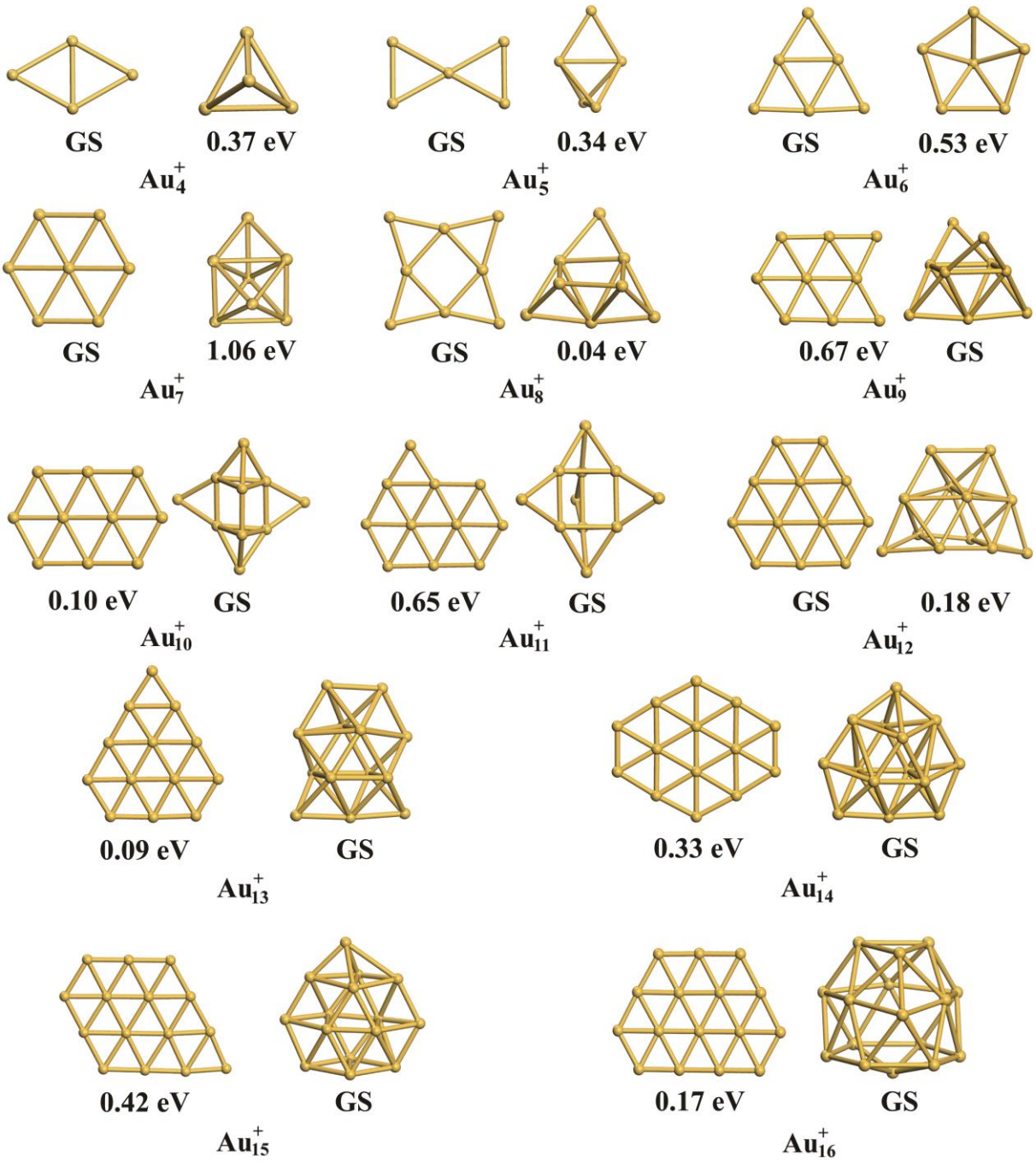


Figure S11 Same as the caption of Fig. S9 except that the above results are calculated by using meta-GGA TPSS functional.

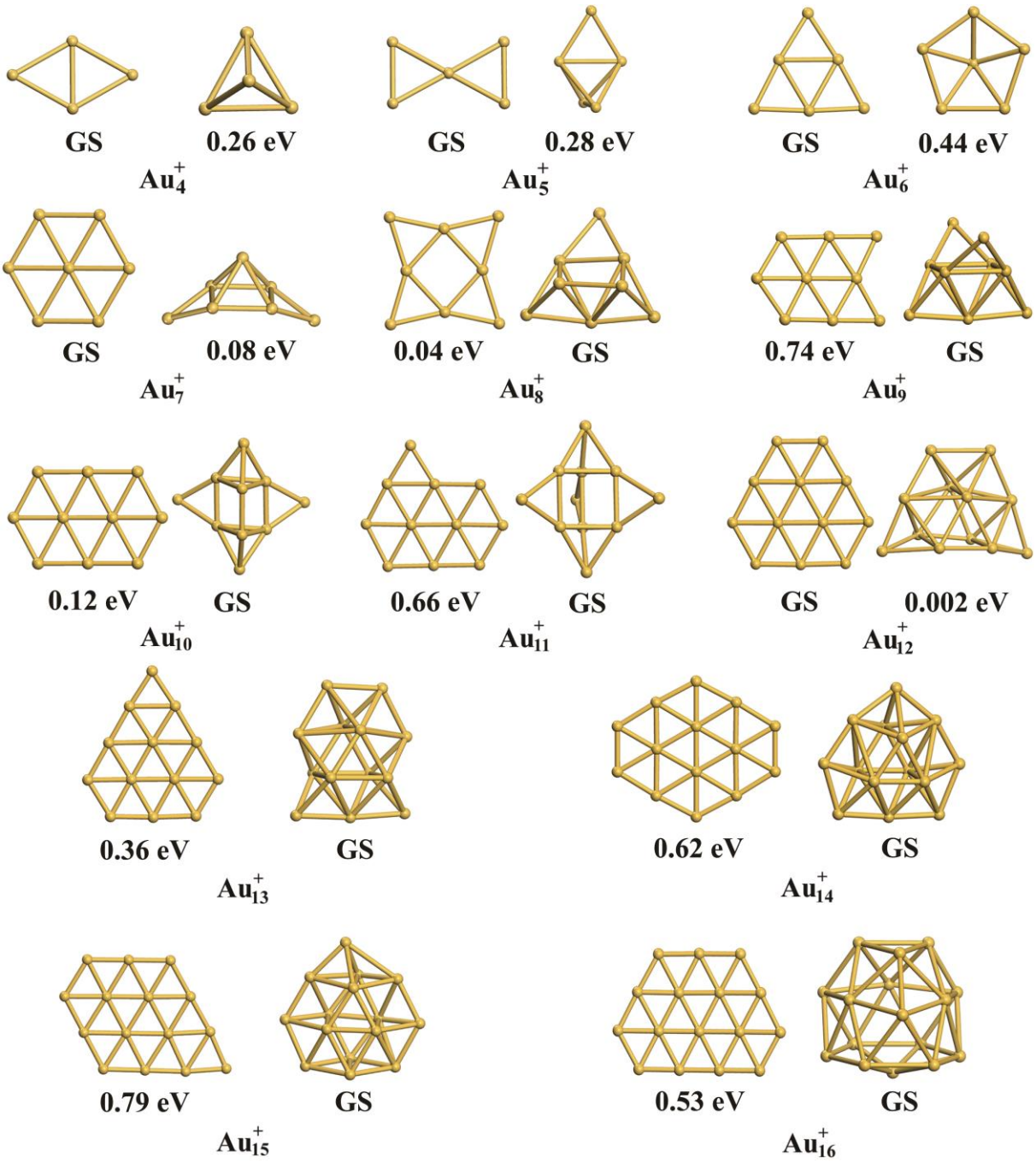


Figure S12 Same as the caption of Fig. S9 except that the above results are calculated by using meta-GGA revTPSS functional.

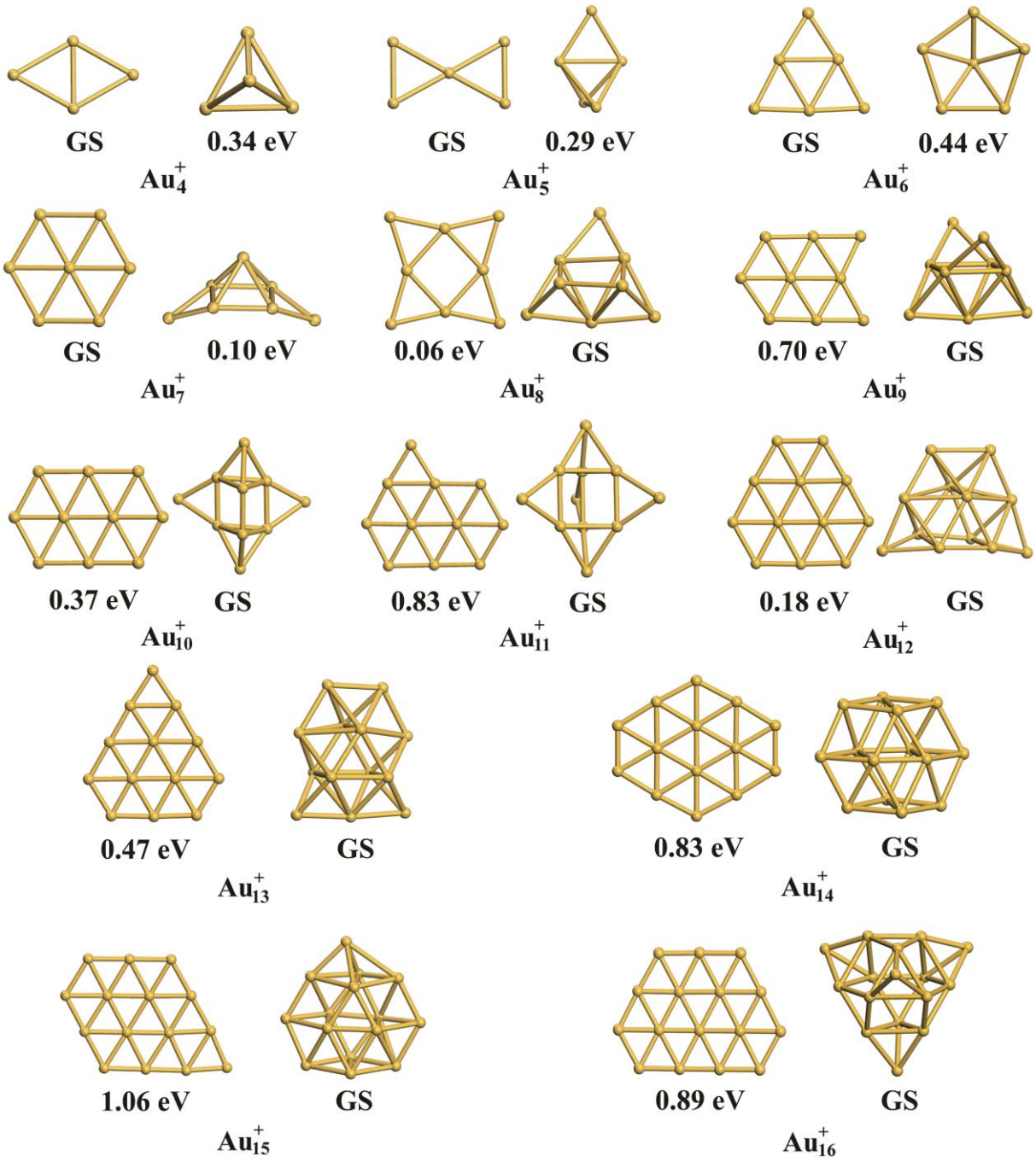
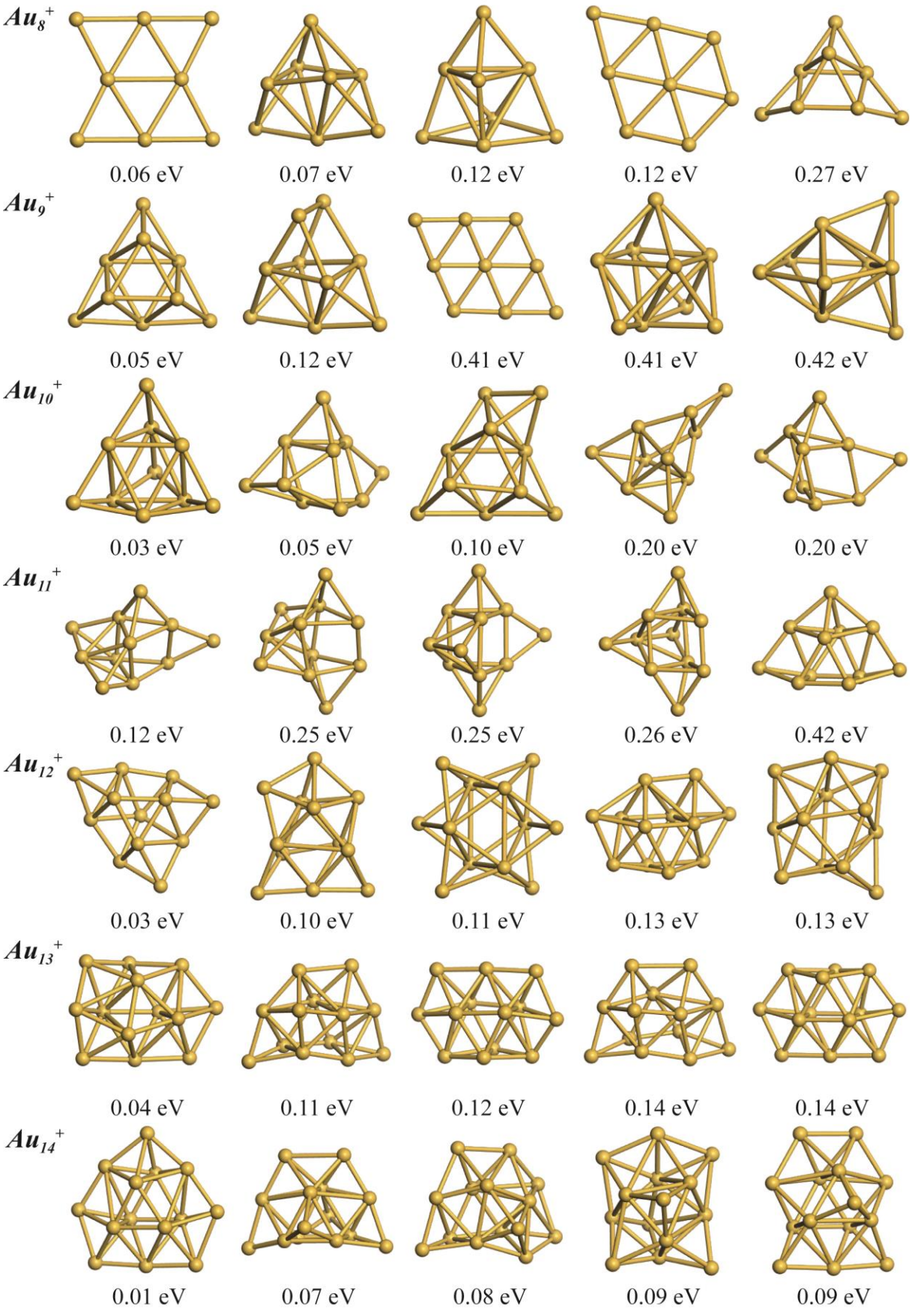


Figure S13 Same as the caption of Fig. S9 except that the above results are calculated by using TSD-PBE method.


Au_8^+
0.06 eV
0.07 eV
0.12 eV
0.12 eV
0.27 eV
Au_9^+
0.05 eV
0.12 eV
0.41 eV
0.41 eV
0.42 eV
Au_{10}^+
0.03 eV
0.05 eV
0.10 eV
0.20 eV
0.20 eV
Au_{11}^+
0.12 eV
0.25 eV
0.25 eV
0.26 eV
0.42 eV
Au_{12}^+
0.03 eV
0.10 eV
0.11 eV
0.13 eV
0.13 eV
Au_{13}^+
0.04 eV
0.11 eV
0.12 eV
0.14 eV
0.14 eV
Au_{14}^+
0.01 eV
0.07 eV
0.08 eV
0.09 eV
0.09 eV

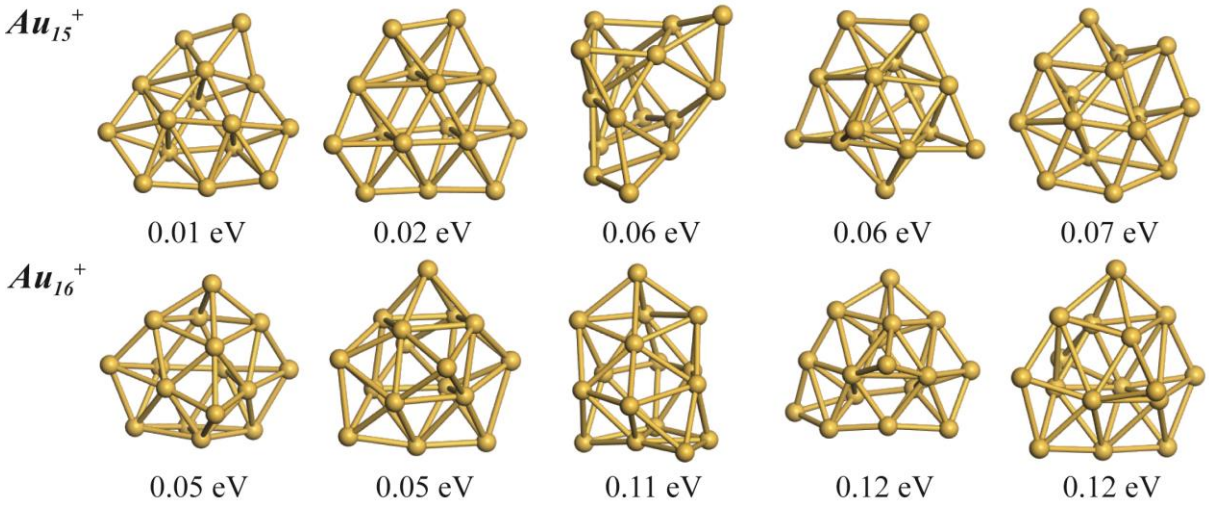


Figure S14 The first 5 low-lying isomers for the Au_n^+ (n≥8) anions calculated by using the TSD-PBE method. The relative energy is provided below the corresponding isomer.

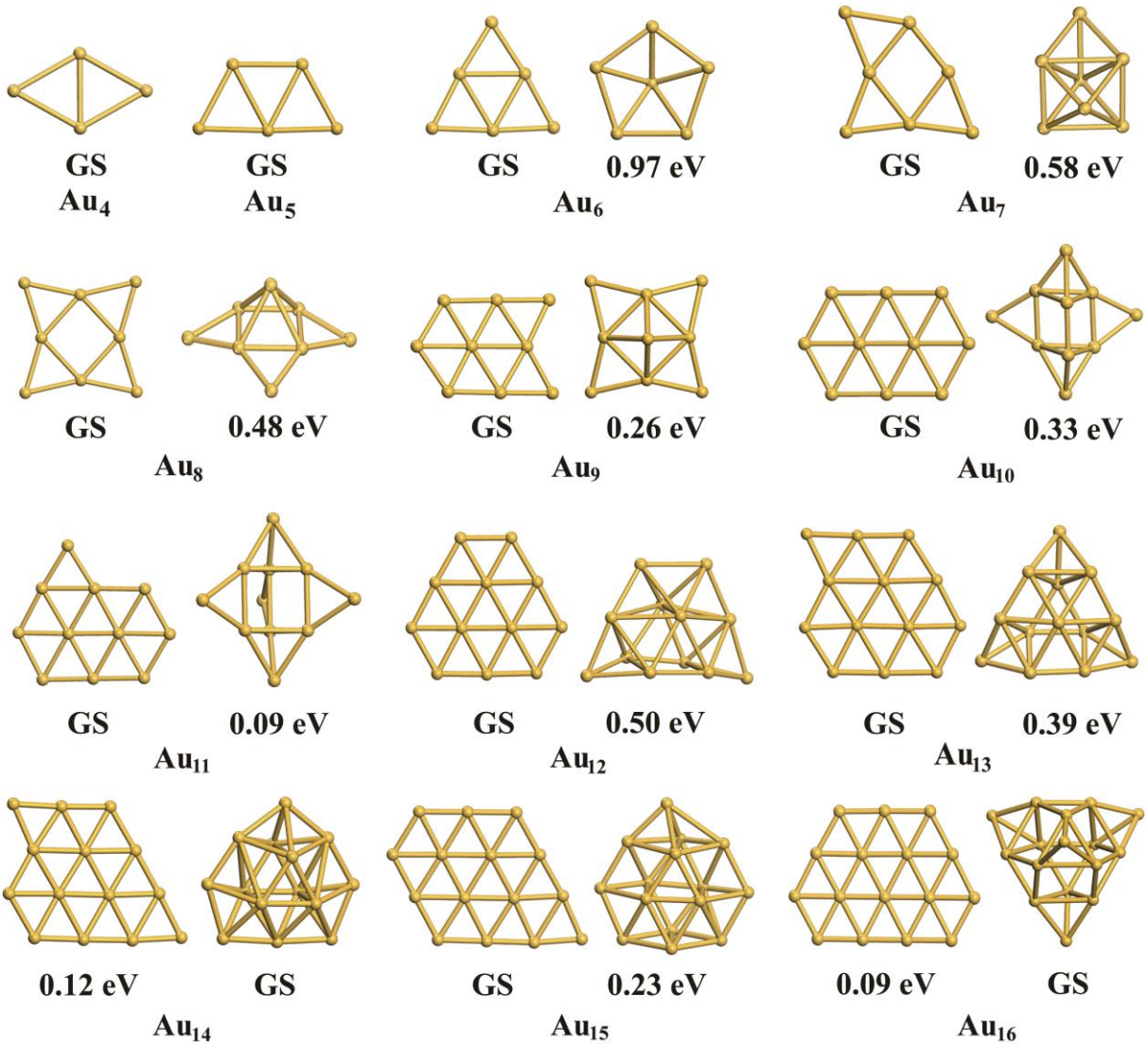


Figure S15 The lowest energy 2D and 3D structures among the corresponding planar and non-planar structures studied by using PBE functional for Au_n neutral clusters, respectively. No 3D compact structures were found in our studies for the Au_4 and Au_5 clusters. The GS stands for the ground state structure. The relative energy is provided below the corresponding isomer.

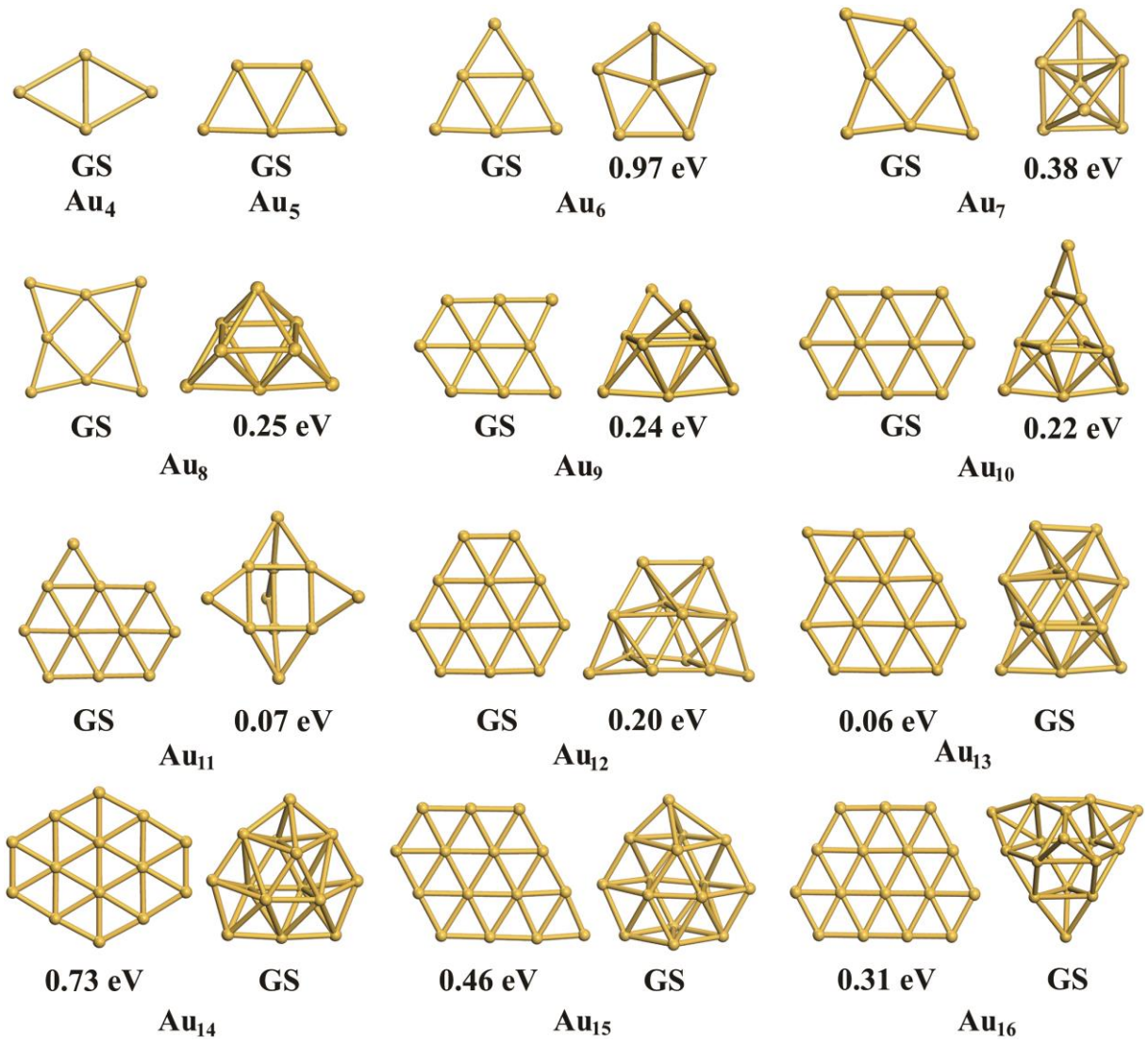


Figure S16 Same as the caption of Fig. S15 except that the above results are calculated by PBEsol functional.

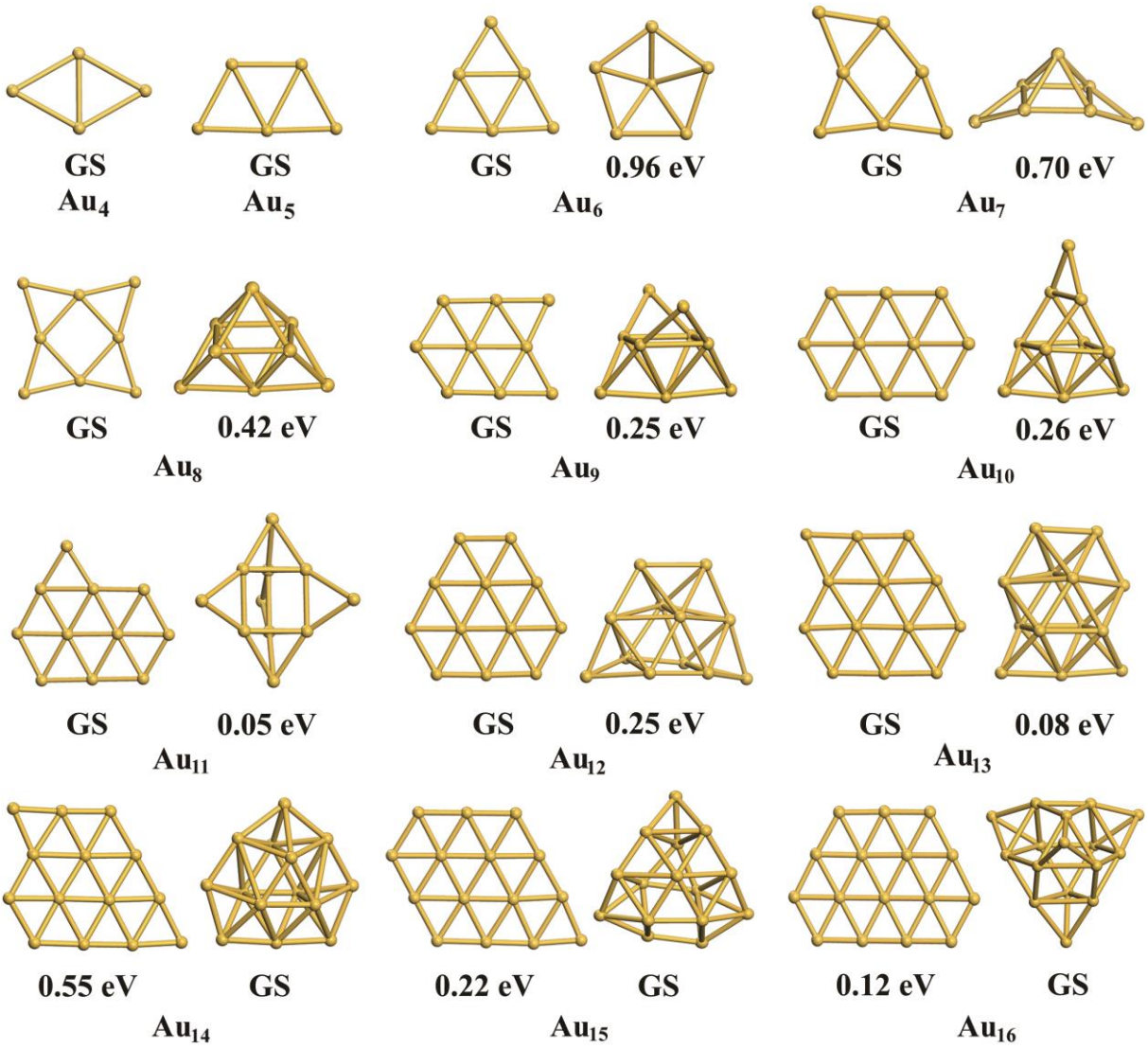


Figure S17 Same as the caption of Fig. S15 except that the above results are calculated by using meta-GGA TPSS functional.

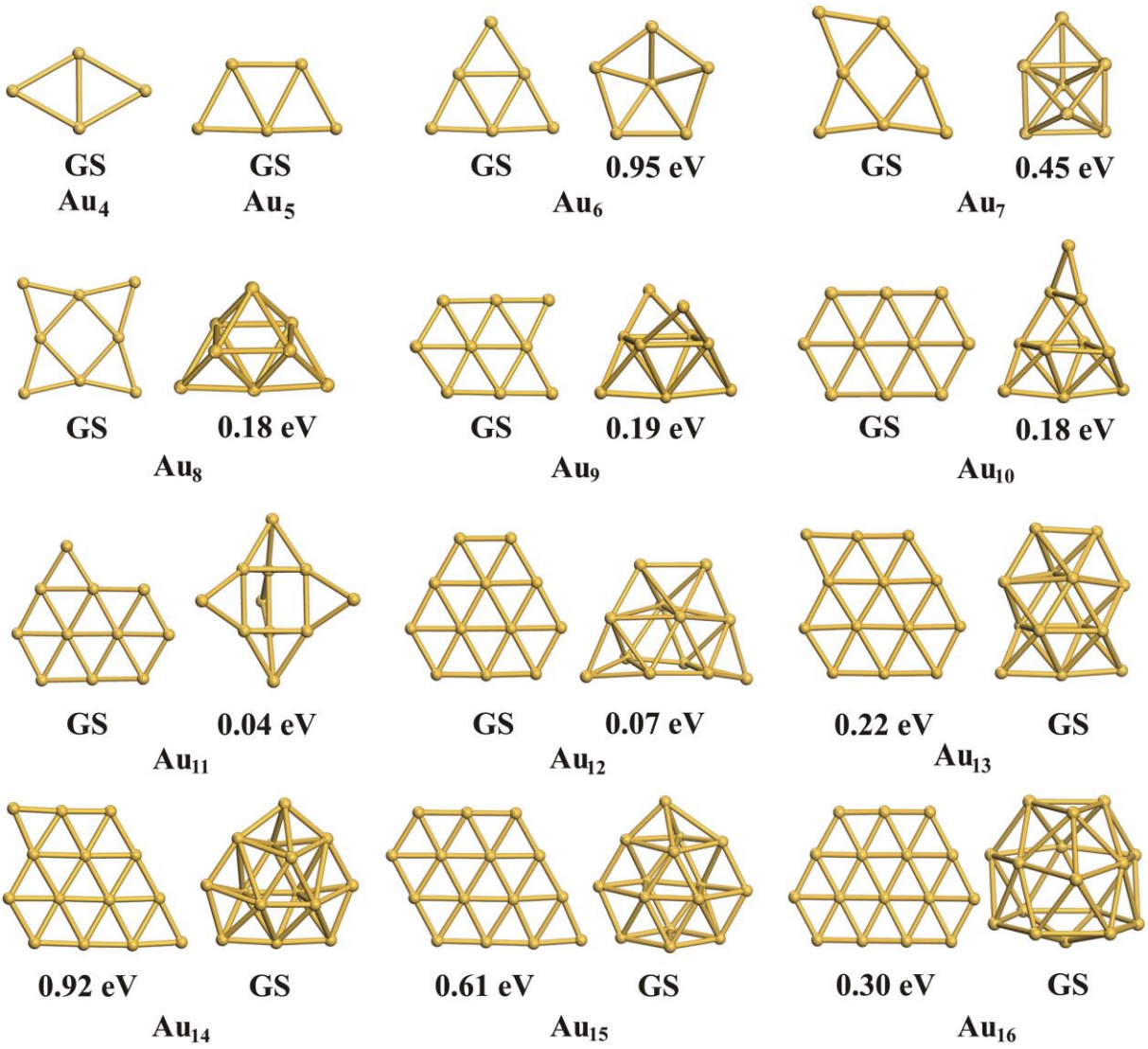


Figure S18 Same as the caption of Fig. S15 except that the above results are calculated by using meta-GGA revTPSS functional.

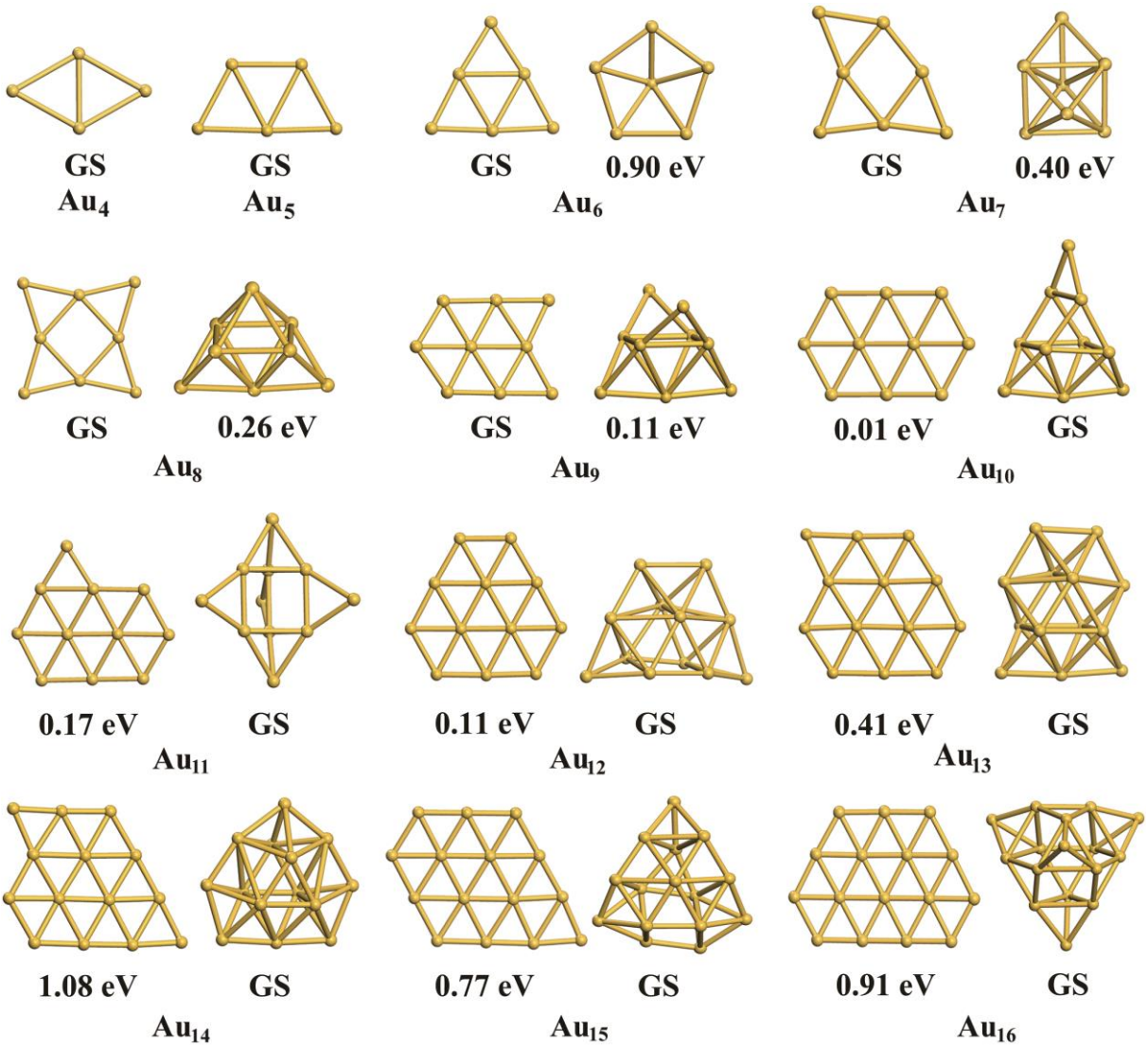


Figure S19 Same as the caption of Fig. S15 except that the above results are calculated by using TSD-PBE method.

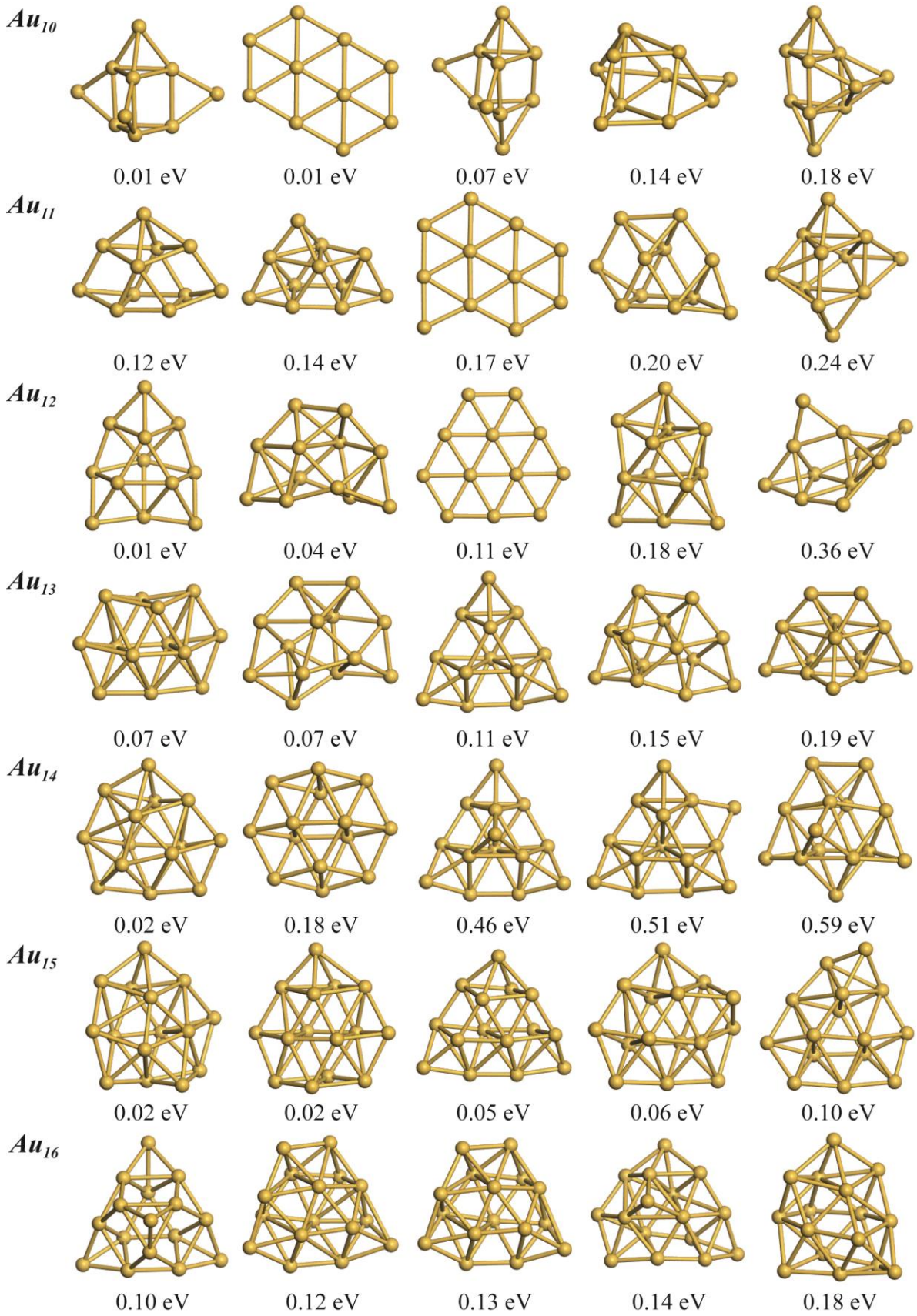


Figure S20 The first 5 low-lying isomers for the Au_n (n≥10) calculated by using the TSD-PBE method. The relative energy is provided below the corresponding isomer.