Supporting Material:

Dopant-induced 2D-3D transition in small Au-containing clusters: DFT-global optimization of 8-atom Au-Ag nanoalloys

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Figures

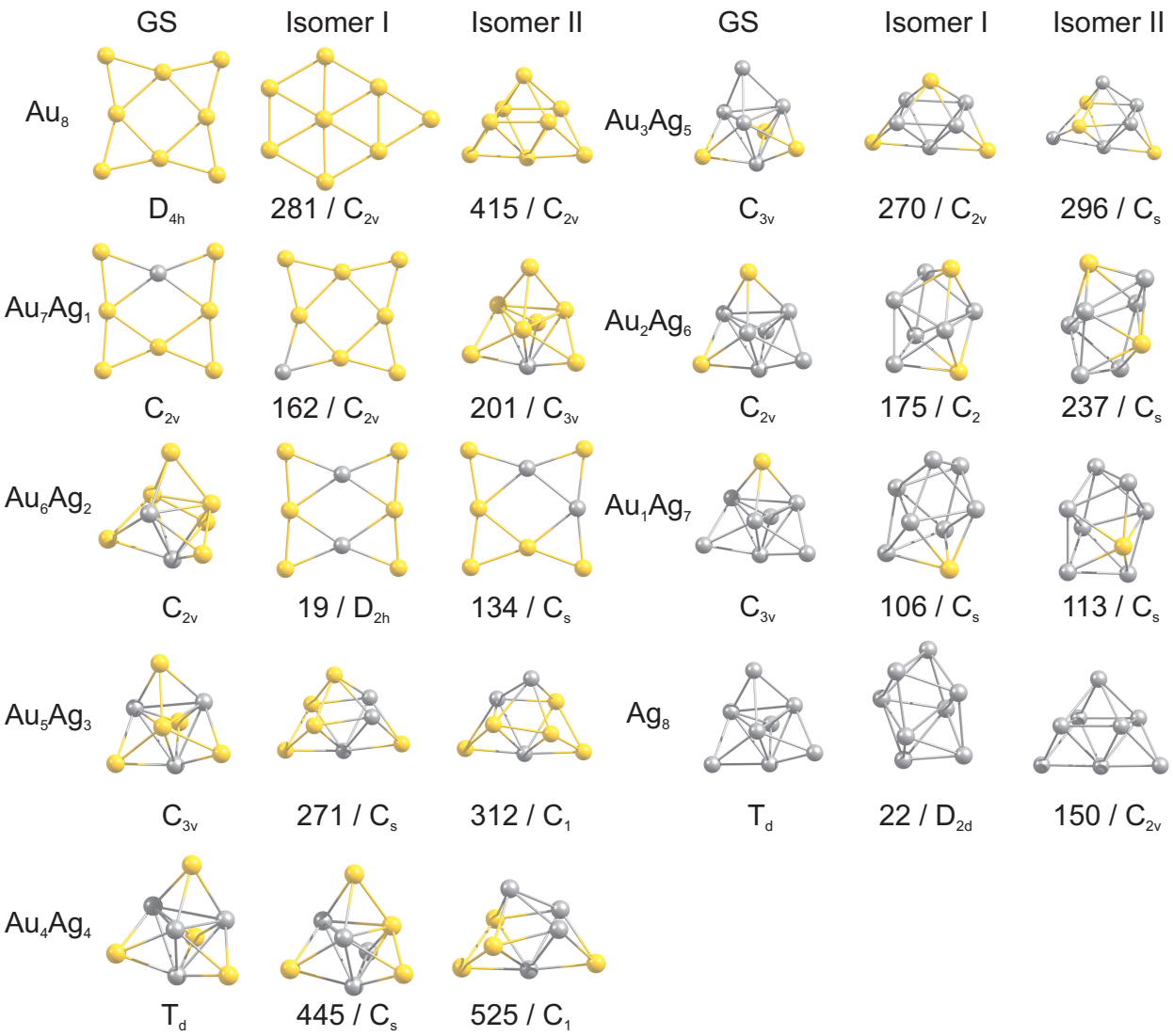

Fig. S 1: The three lowest lying isomers after reoptimization with QE. For all isomers the point group and for higher lying isomers the energy difference in meV with respect to the GS is given.

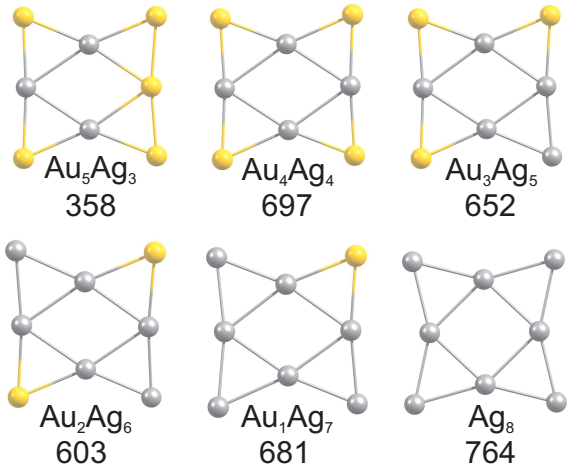

Fig. S 2: The three lowest lying 2D isomers after reoptimization with QE. Below each isomer the energy difference to the GS is given in meV.

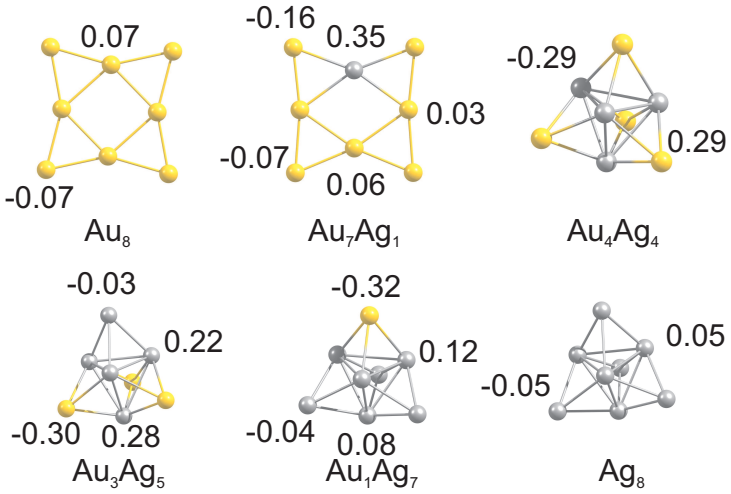

Fig. S 3: The Bader charges are given for all non-symmetry equivalent atoms for some pure and doped GS isomers in atomic units.