Supporting Information

Argon adsorption on cationic gold clusters Au_n^+ ($n \leq 20$)

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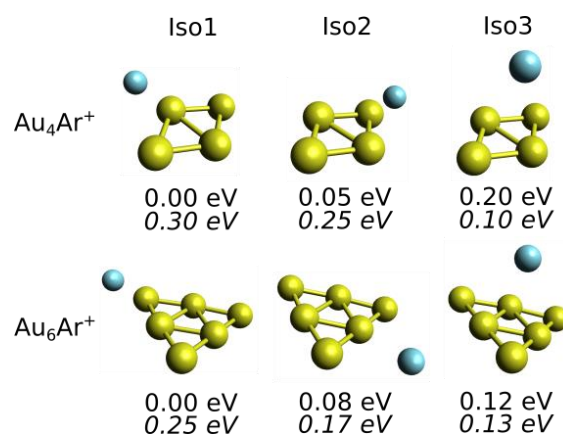1. Ar adsorption site isomers of Au_4Ar^+ and Au_6Ar^+

Figure S1. Ar adsorption site isomers of Au_4Ar^+ and Au_6Ar^+ clusters. The energies relative to the lowest energy adsorption site are presented below each structure, as well as the Ar adsorption energy (E_{ads}, in italics) of each isomer.

2. Optimized geometries of $Au_nAr_m^+$ ($n = 3 – 20$; $m = 1 - 5$) clusters

The coordinates of those clusters are available through Github at https://github.com/pferrari13/Au_nAr_m-XYZ-coordinates.git
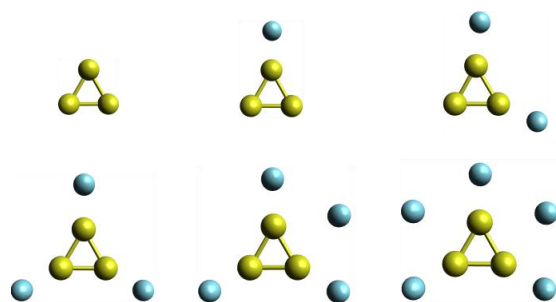

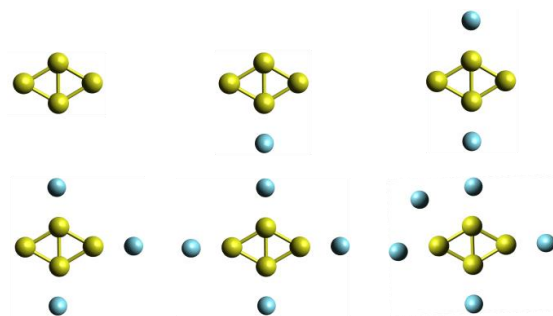Figure S2. Optimized geometries of $Au_3Ar_m^+$ ($m = 0-5$).

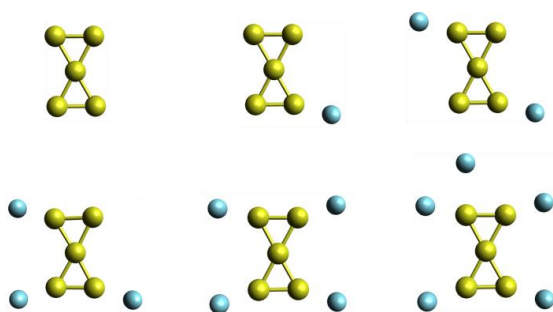Figure S3. Optimized geometries of $Au_4Ar_m^+$ (m = 0-5).

Figure S4. Optimized geometries of $Au_5Ar_m^+$ (m = 0-5).
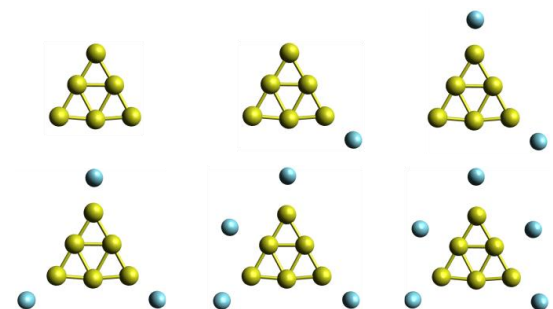

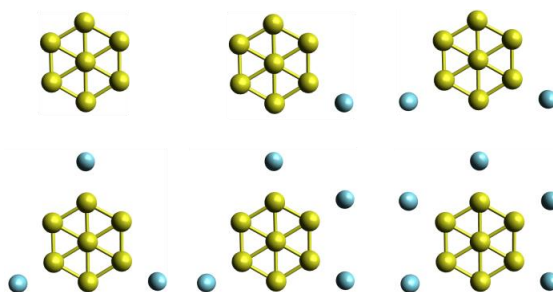Figure S5. Optimized geometries of $Au_6Ar_m^+$ (m = 0-5).
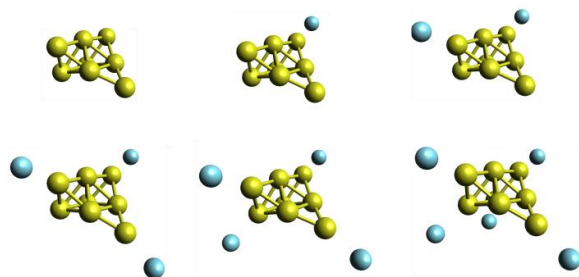

Figure S6. Optimized geometries of $Au_7Ar_m^+$ (m = 0-5).

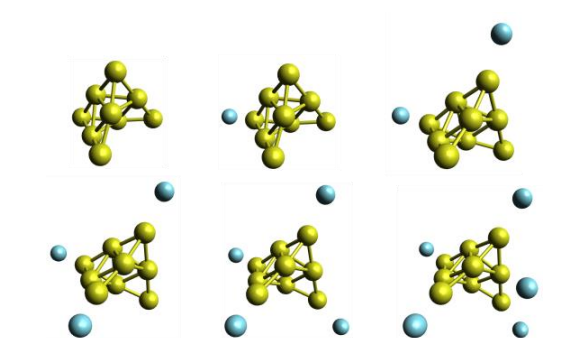Figure S7. Optimized geometries of $Au_8Ar_m^+$ (m = 0-5).

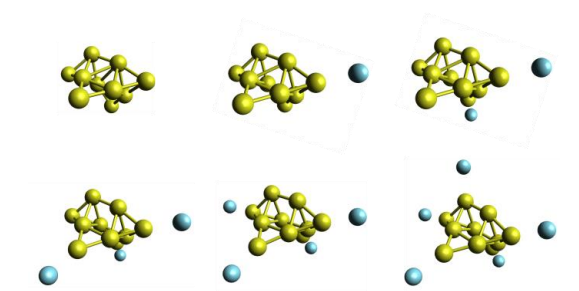Figure S8. Optimized geometries of $Au_9Ar_m^+$ (m = 0-5).

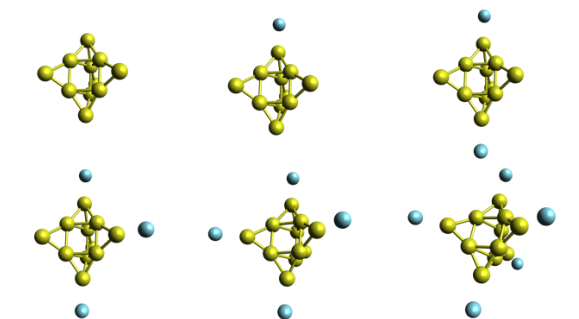Figure S9. Optimized geometries of $Au_{10}Ar_m^+$ (m = 0-5).

Figure S10. Optimized geometries of $Au_{11}Ar_m^+$ (m = 0-5).

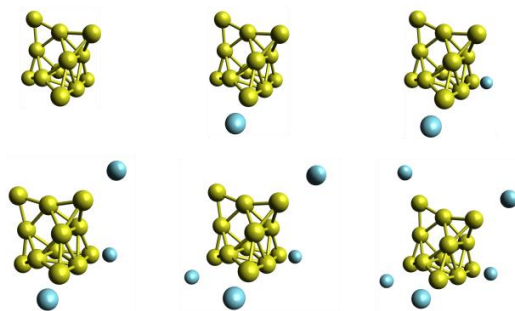Figure S11. Optimized geometries of $Au_{12}Ar_m^+$ (m = 0-5).

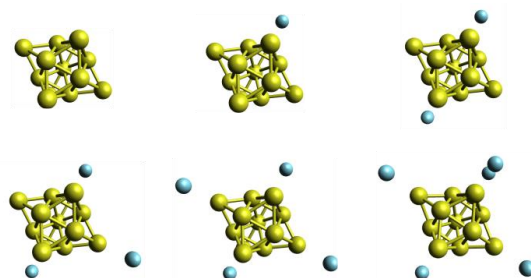Figure S12. Optimized geometries of $Au_{13}Ar_m^+$ (m = 0-5).

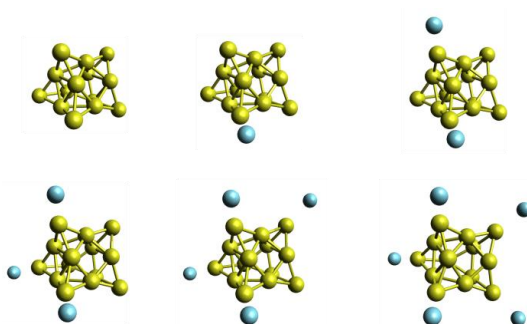Figure S13. Optimized geometries of $Au_{14}Ar_m^+$ (m = 0-5).
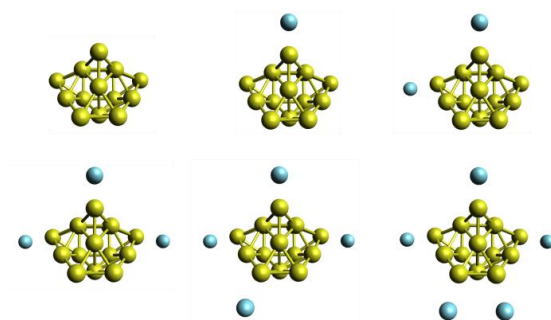

Figure S14. Optimized geometries of $Au_{15}Ar_m^+$ (m = 0-5).
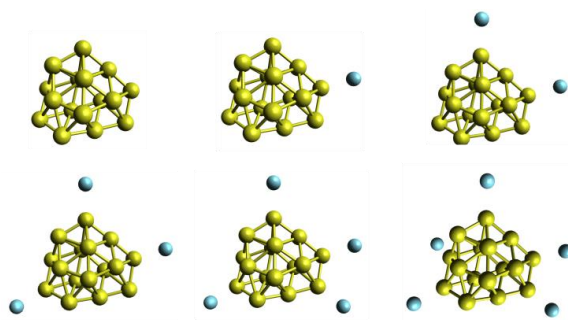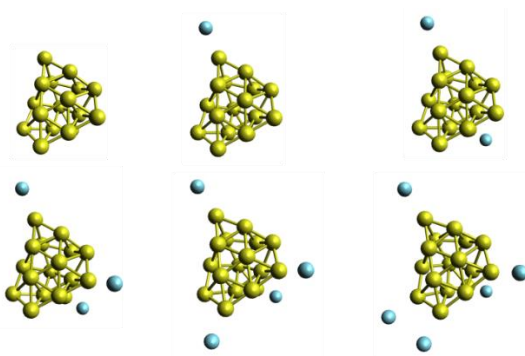
Figure S15. Optimized geometries of $Au_{16}Ar_m^+$ (m = 0-5).
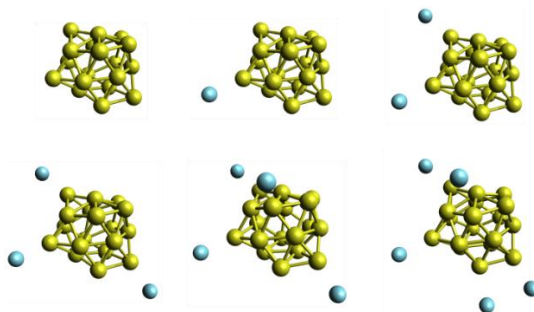

Figure S16. Optimized geometries of $Au_{17}Ar_m^+$ (m = 0-5).
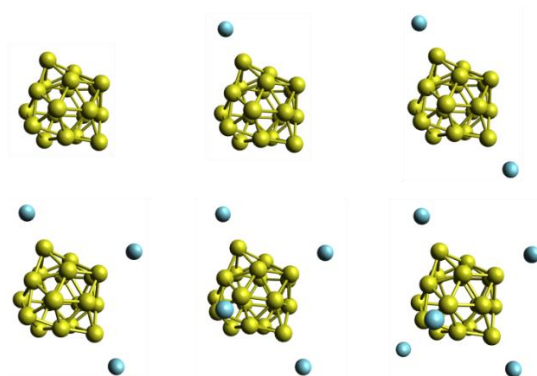

Figure S17. Optimized geometries of $Au_{18}Ar_m^+$ (m = 0-5).
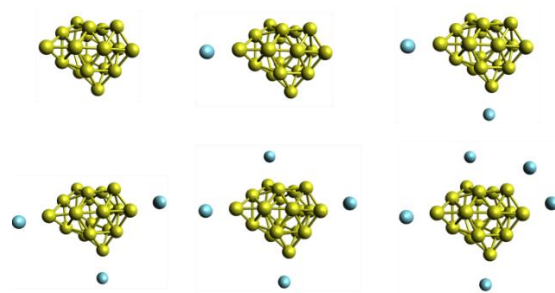

Figure S18. Optimized geometries of $Au_{19}Ar_m^+$ (m = 0-5).

Figure S19. Optimized geometries of $Au_{20}Ar_m^+$ (m = 0-5).