

The Effect of Spin Multiplicity in O₂ Adsorption and Dissociation on Small Bimetallic AuAg Clusters

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Supporting information

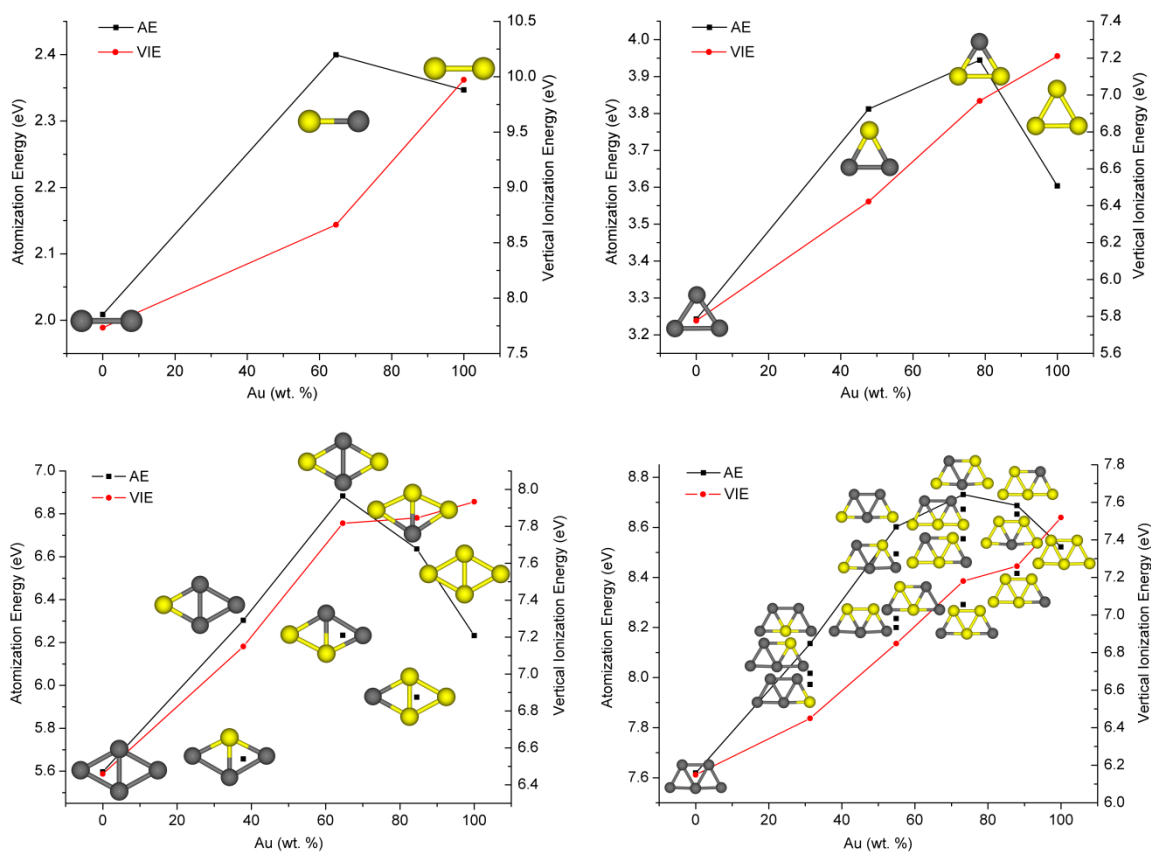


Figure S1 Characterization of Au_nAg_m ($n + m \leq 5$) clusters in terms of Au wt. %. Vertical ionization energy corresponds to most stable AuAg clusters.

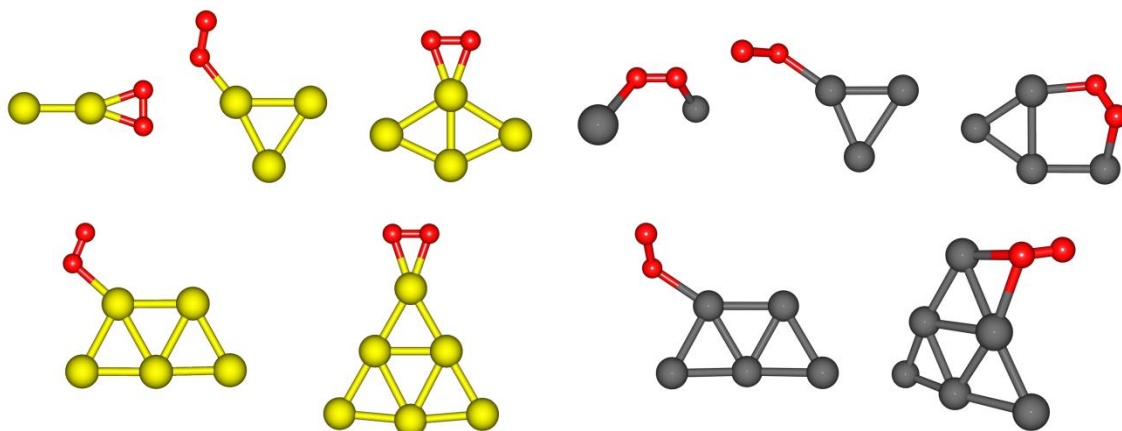


Figure S2. Most stable Au_nO_2 and Ag_mO_2 ($n, m \leq 6$) adducts obtained at PBE/TZVP/ZORA level of theory with spin multiplicities singlet ($n, m = 2, 4$, and 6) and quartet ($n, m = 3$ and 5).

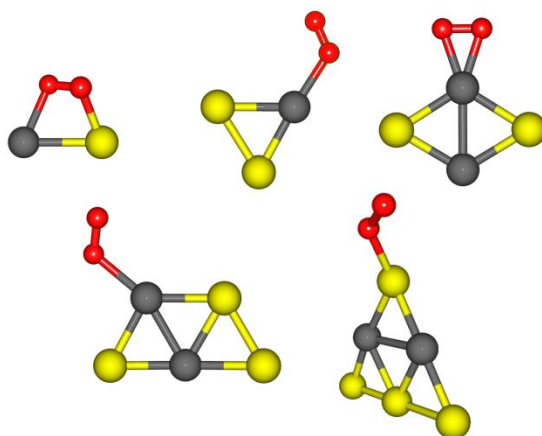


Figure S3 Most stable $\text{Au}_n\text{Ag}_m\text{O}_2$ adducts obtained at PBE/TZVP/ZORA level of theory with spin multiplicities singlet ($n + m = 2, 4$, and 6) and quartet ($n + m = 3$ and 5).

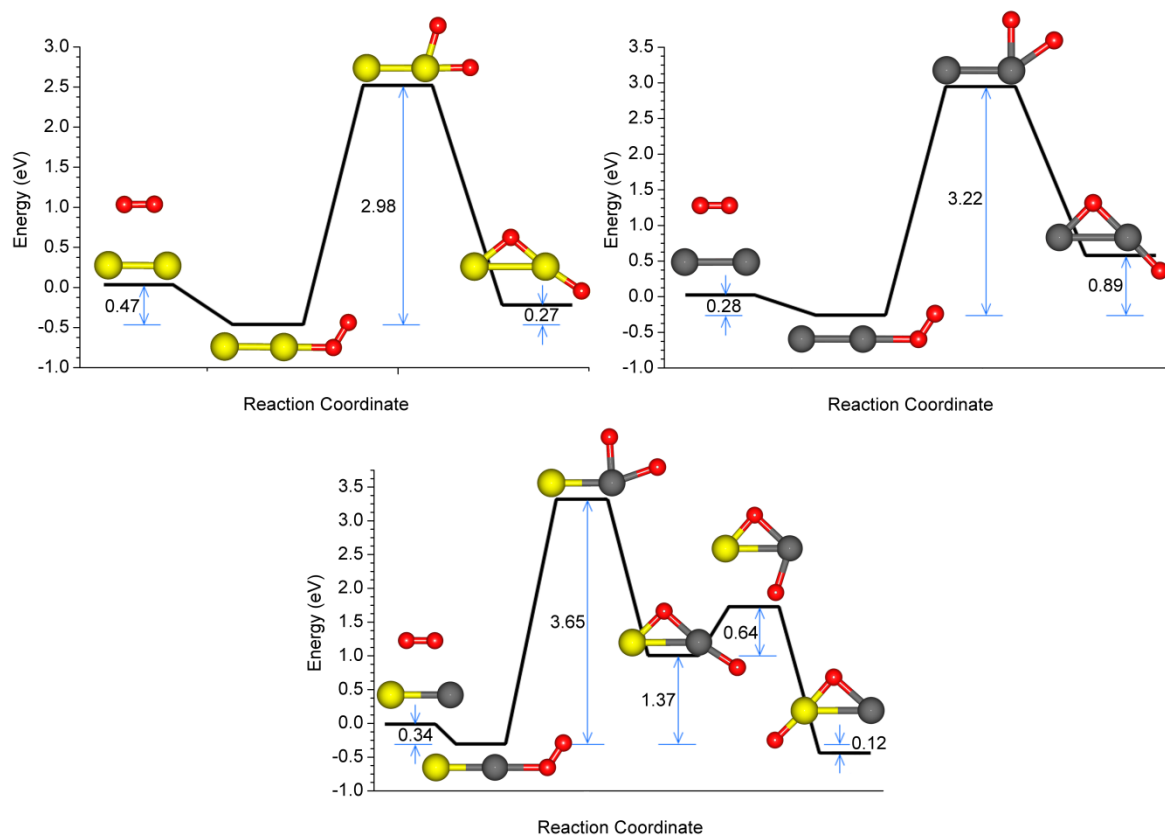


Figure S4 Energy profile of the O_2 dissociation on pure and bimetallic clusters with two atoms. Results obtained at PBE/TZVP/ZORA level of theory.

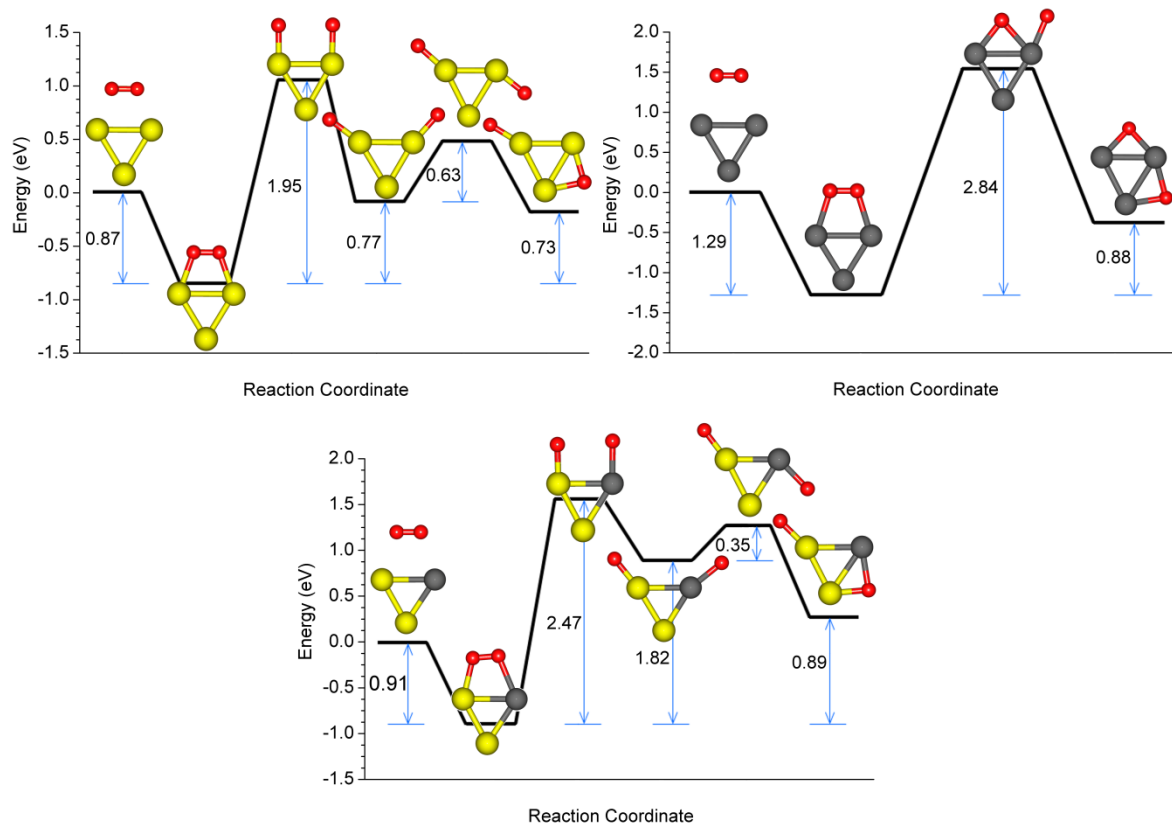


Figure S5 Energy profile of the O_2 dissociation on pure and bimetallic clusters with three atoms. Results obtained at PBE/TZVP/ZORA level of theory.

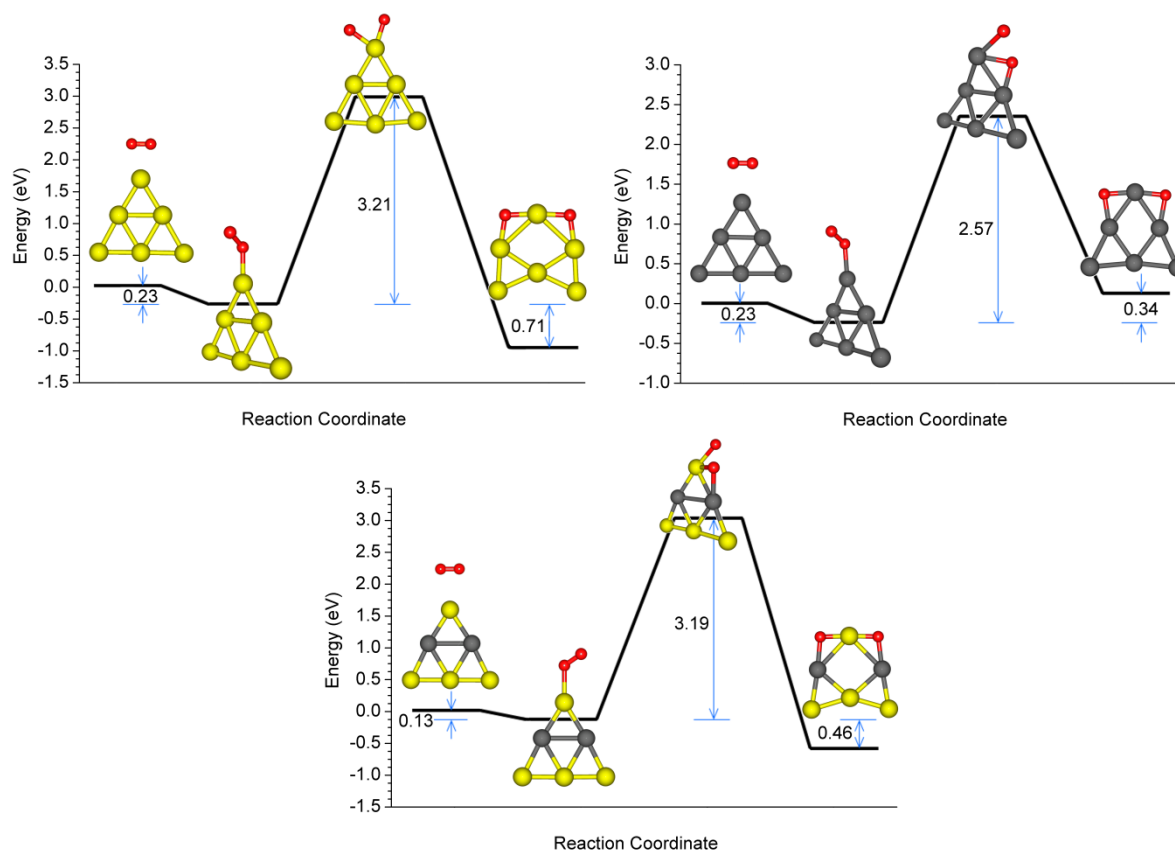


Figure S6 Energy profile of the O_2 dissociation on pure and bimetallic clusters with six atoms. Results obtained at PBE/TZVP/ZORA level of theory.