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Supporting Information

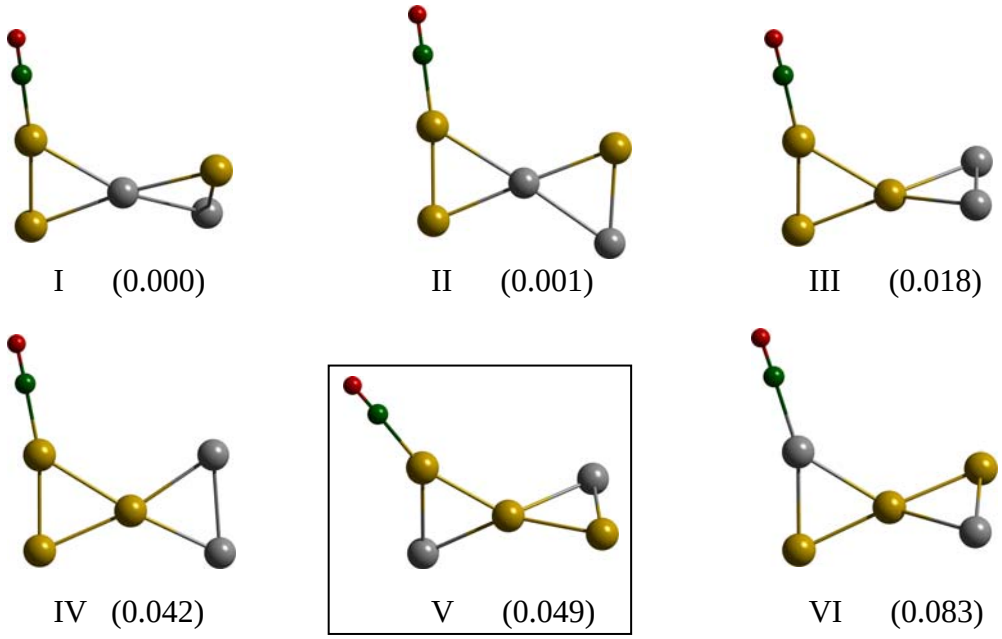


Figure S1: The lowest energy isomers of $Ag_2Au_3CO^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer V shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

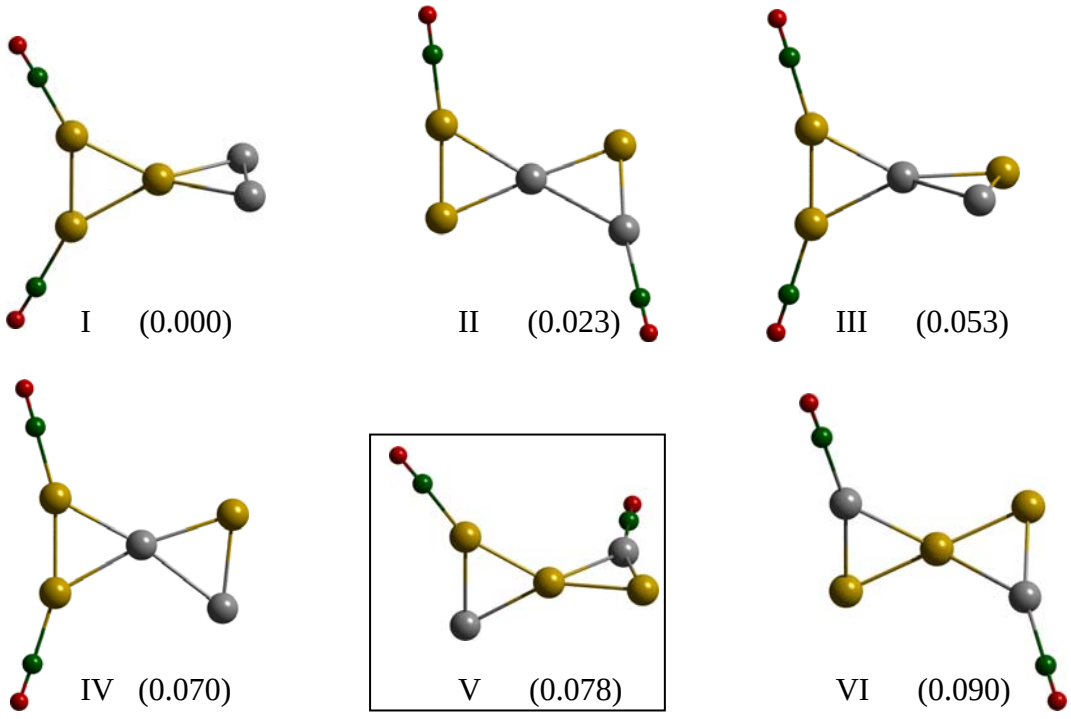


Figure S2: The lowest energy isomers of $Ag_2Au_3(CO)_2^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer V shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

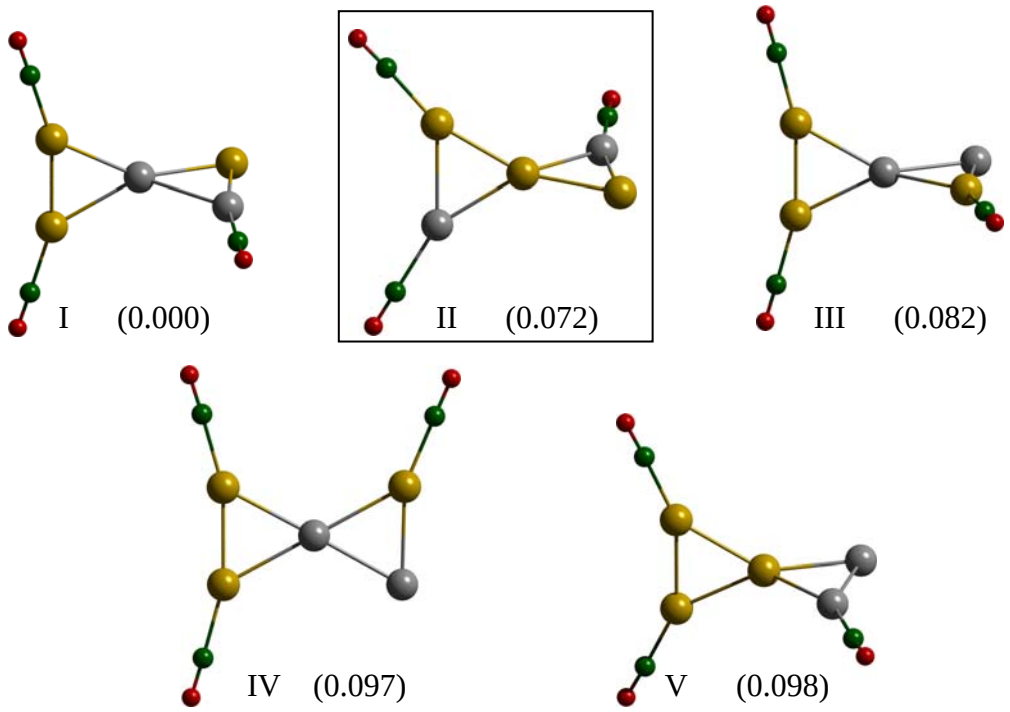


Figure S3: The lowest energy isomers of $Ag_2Au_3(CO)_3^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer II shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

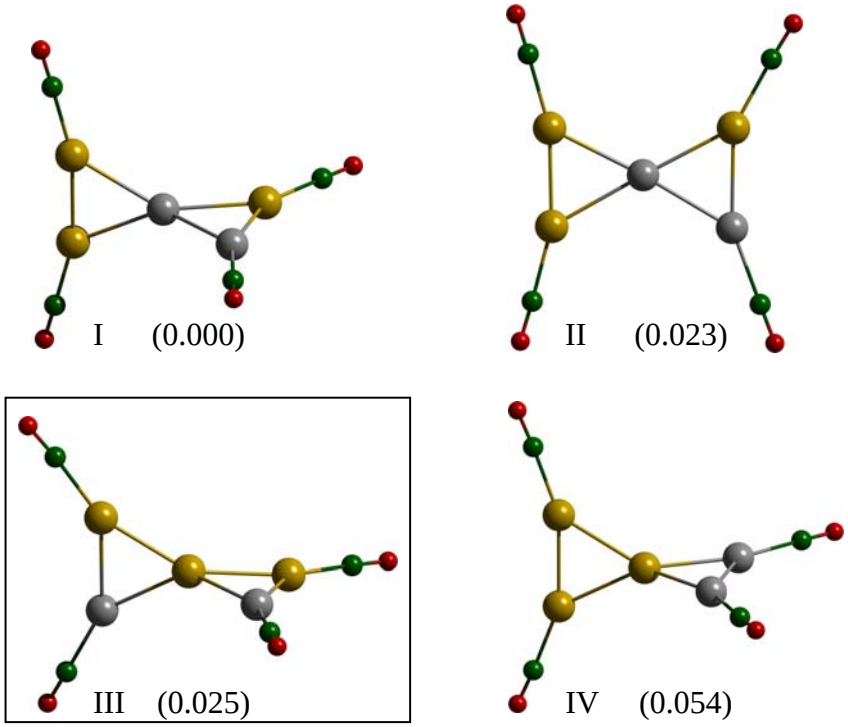


Figure S4: The lowest energy isomers of $Ag_2Au_3(CO)_4^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer III shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

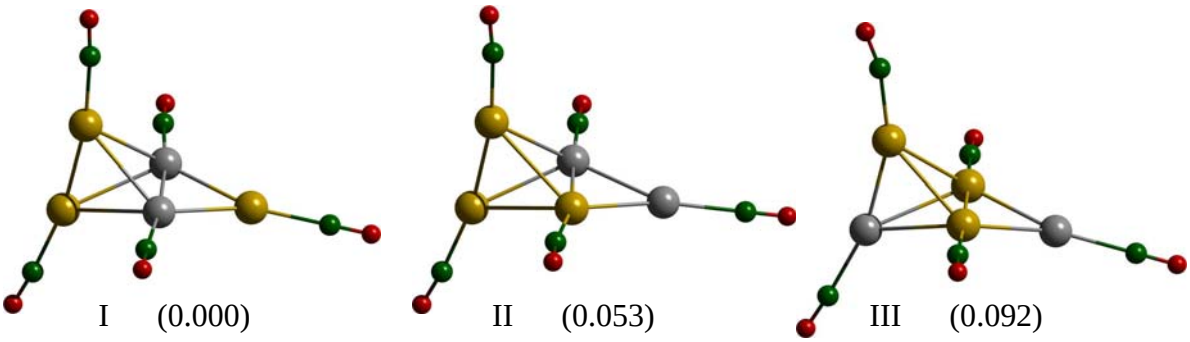
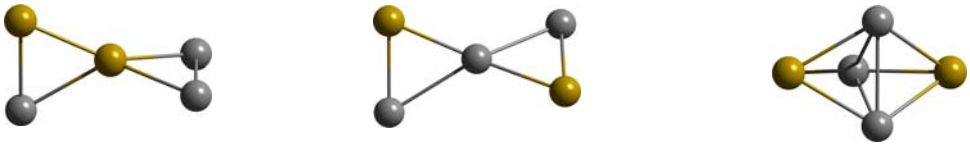
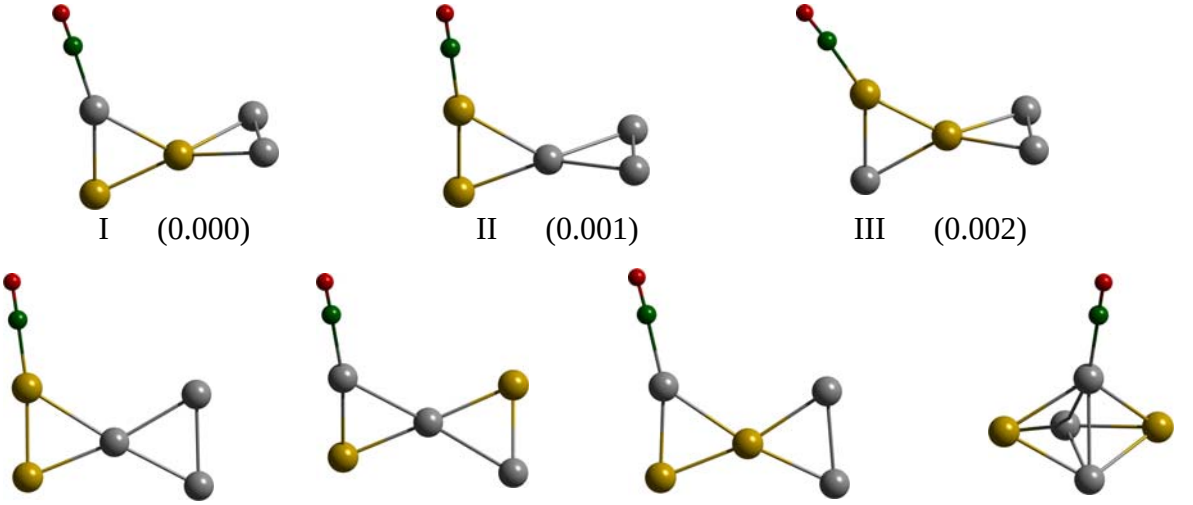


Figure S5: The lowest energy isomers of $Ag_2Au_3(CO)_5^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set.



I (0.000) II (0.044) III (0.054)

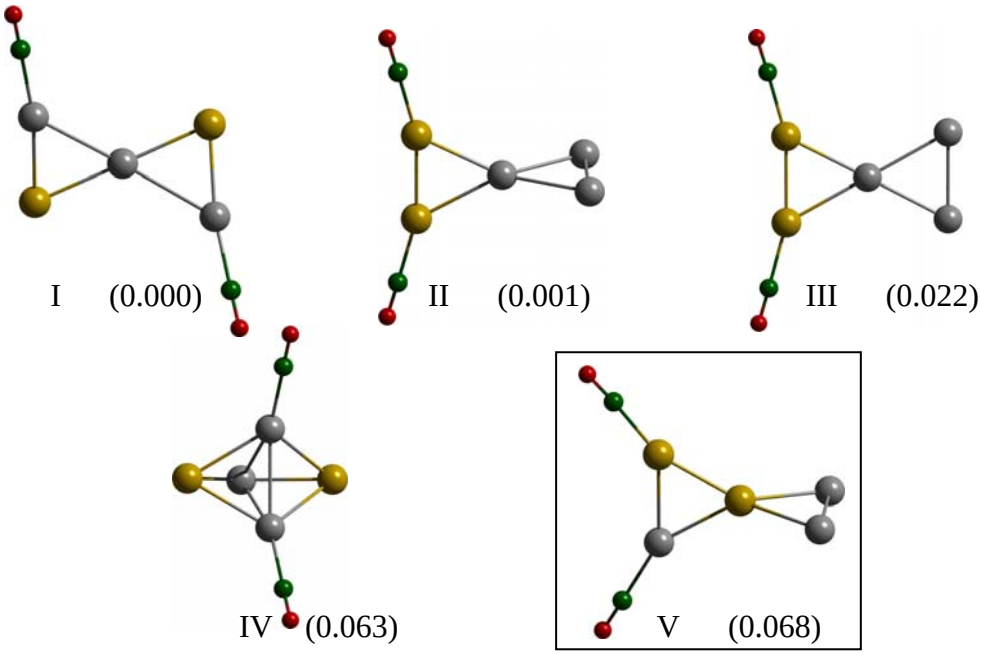
Figure S6: The lowest energy isomers of $Ag_3Au_2^+$ obtained from DFT with B3LYP functional and TZVP atomic basis set. All other isomers are more than 0.2 eV less stable.



I (0.000) II (0.001) III (0.002)

IV (0.016) V (0.034) VI (0.045) VII (0.062)

Figure S7: The lowest energy isomers of $Ag_3Au_2CO^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set.



I (0.000) II (0.001) III (0.022)

IV (0.063) V (0.068)

Figure S8: The lowest energy isomers of $Ag_3Au_2(CO)_2^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer V shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

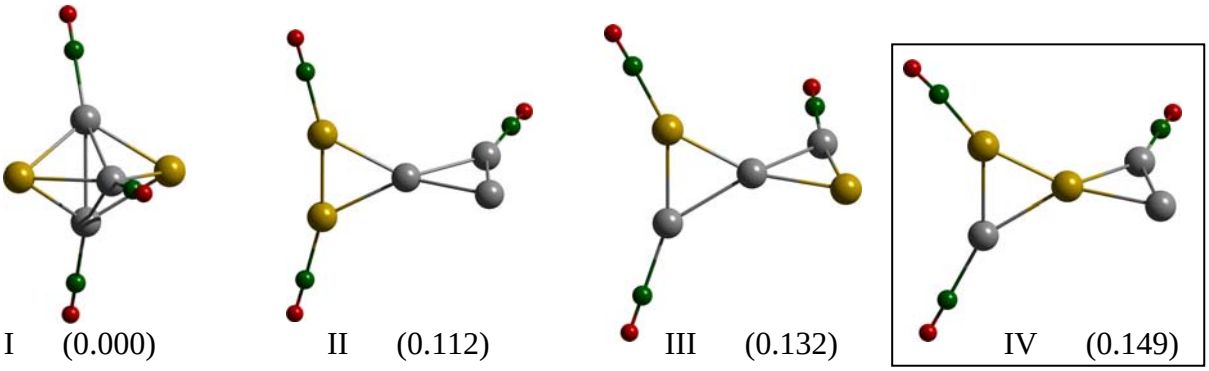


Figure S9: The lowest energy isomers of $Ag_3Au_2(CO)_3^+$ within 0.15 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer IV shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

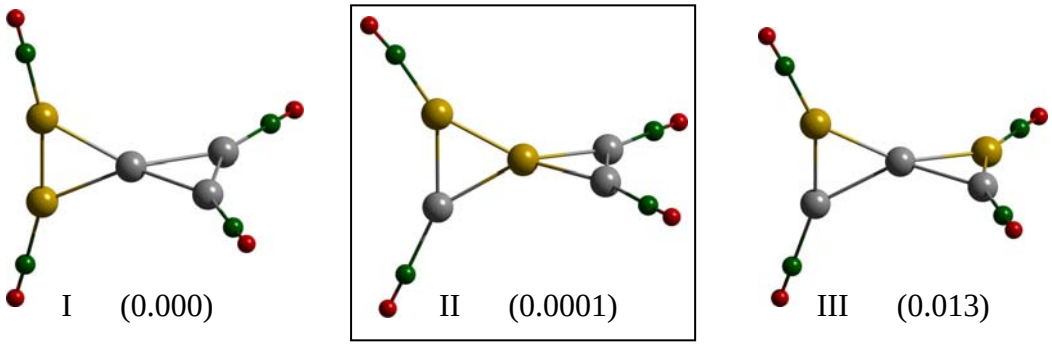


Figure S10: The lowest energy isomers of $Ag_3Au_2(CO)_4^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer II shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

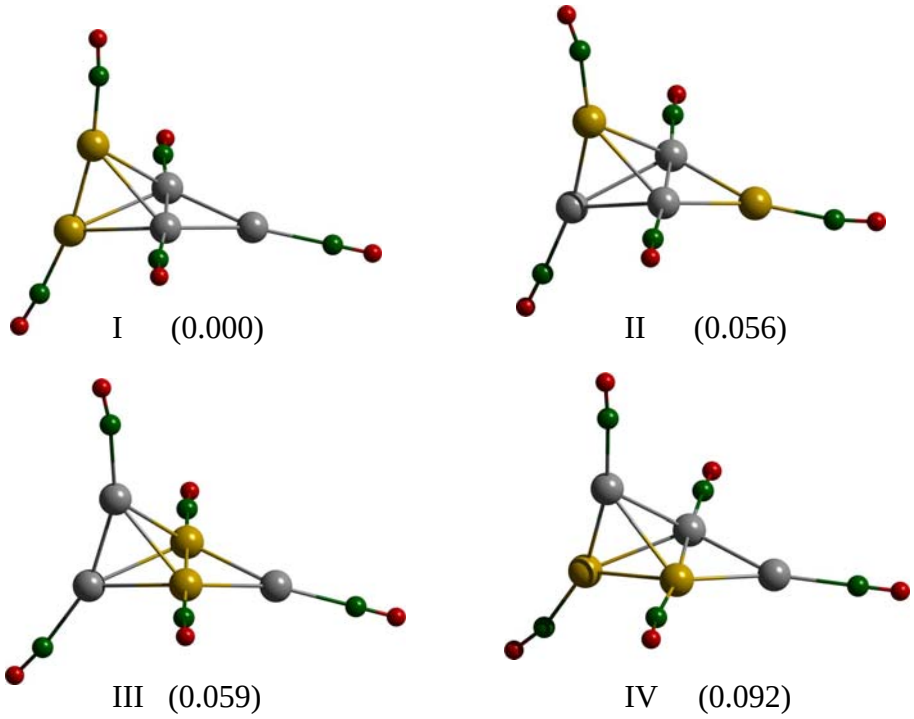


Figure S11: The lowest energy isomers of $Ag_3Au_2(CO)_5^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set.

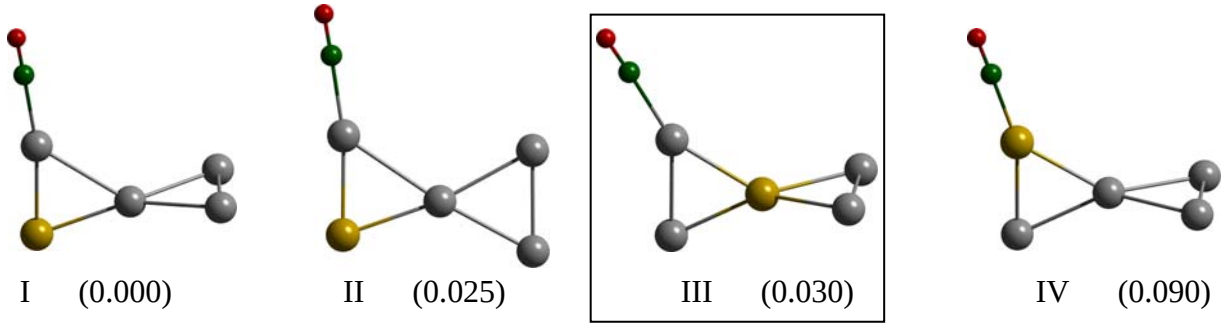


Figure S12: The lowest energy isomers of Ag_4AuCO^+ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer III shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

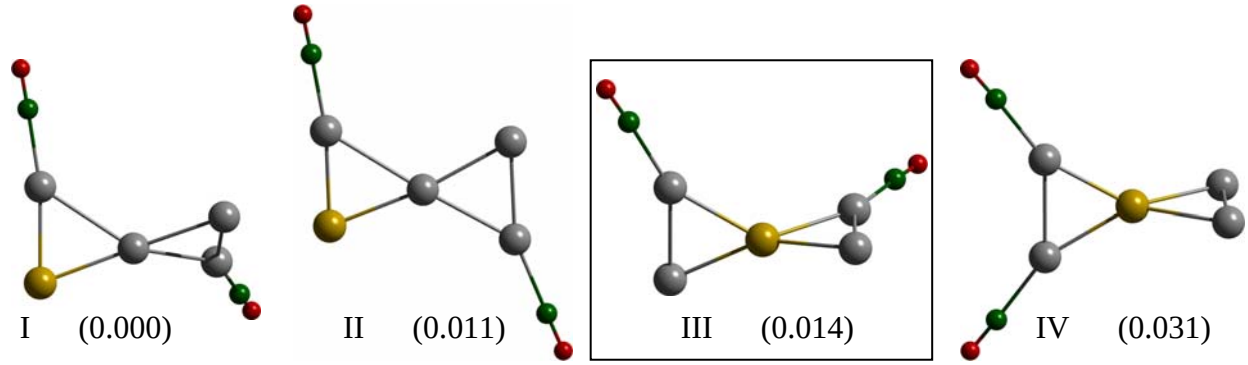


Figure S13: The lowest energy isomers of $Ag_4Au(CO)_2^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer III shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

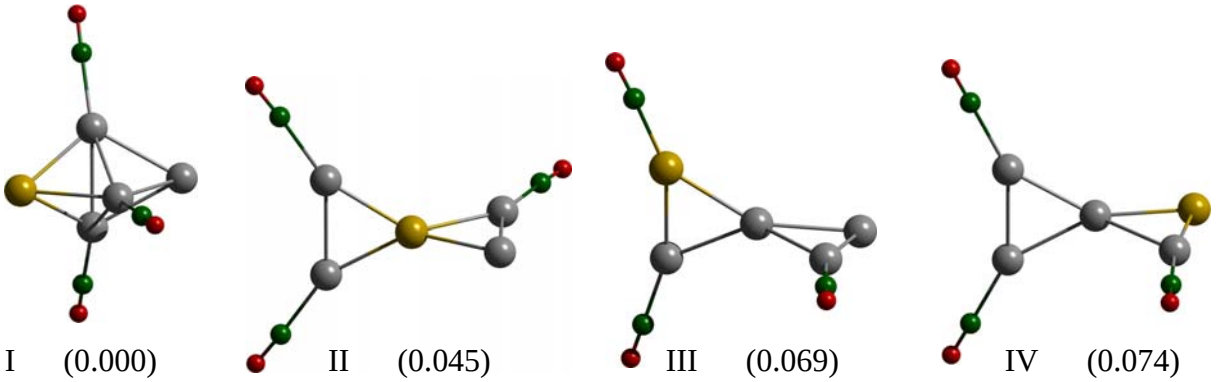


Figure S14: The lowest energy isomers of $Ag_4Au(CO)_3^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set.

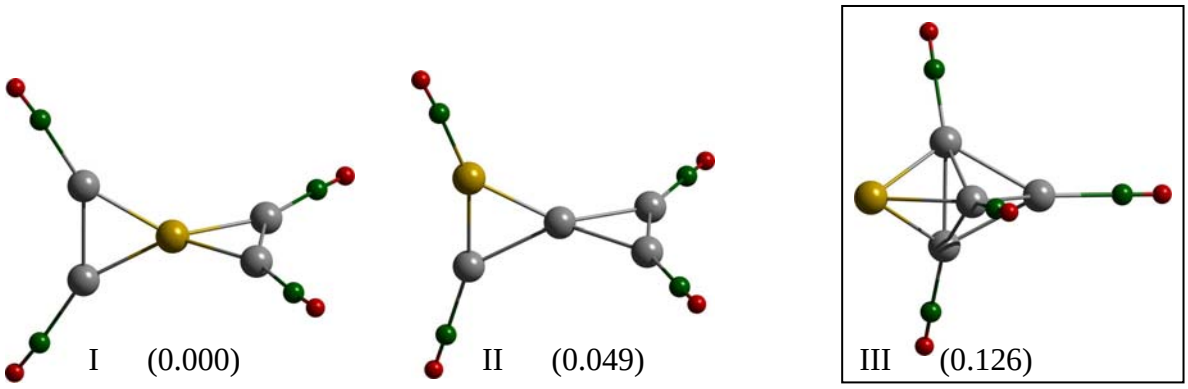


Figure S15: The lowest energy isomers of $Ag_4Au(CO)_4^+$ within 0.13 eV obtained from DFT with B3LYP functional and TZVP atomic basis set. Notice that isomer III shown in window is used in Fig. 5 to illustrate the sequential adsorption of CO.

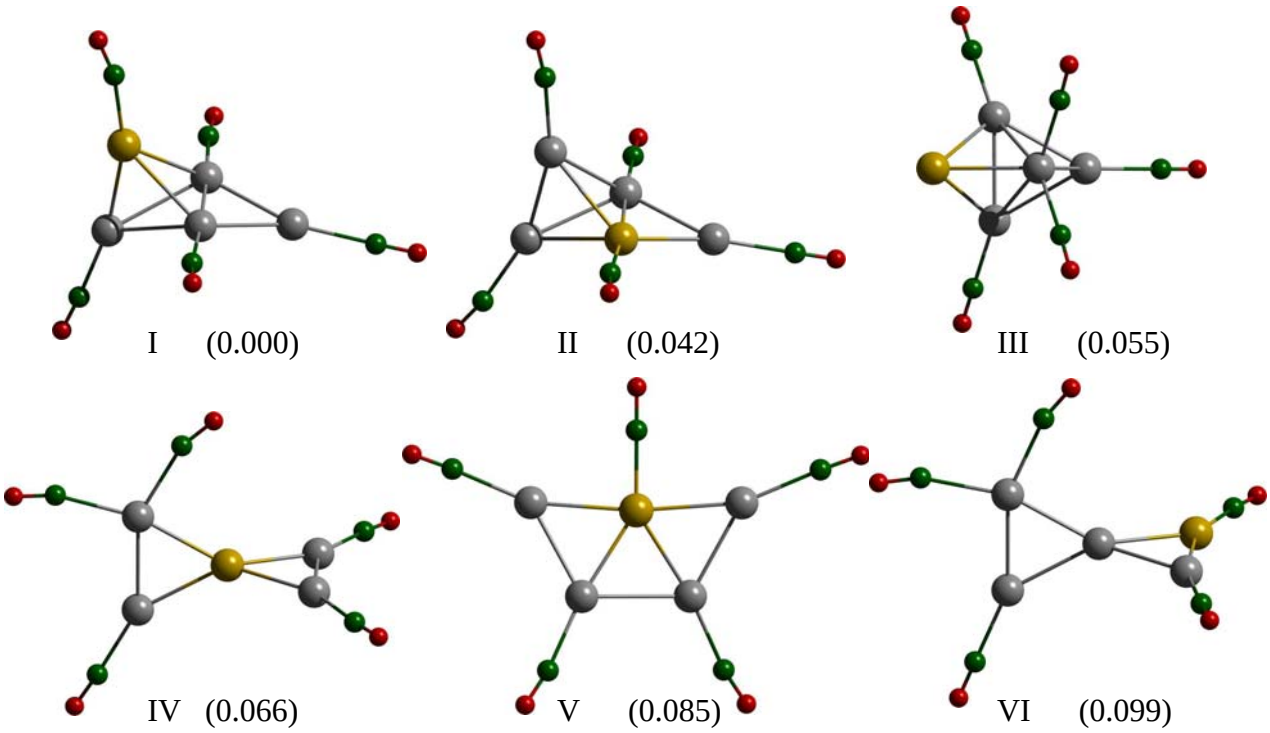


Figure S16: The lowest energy isomers of $Ag_4Au(CO)_5^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set.

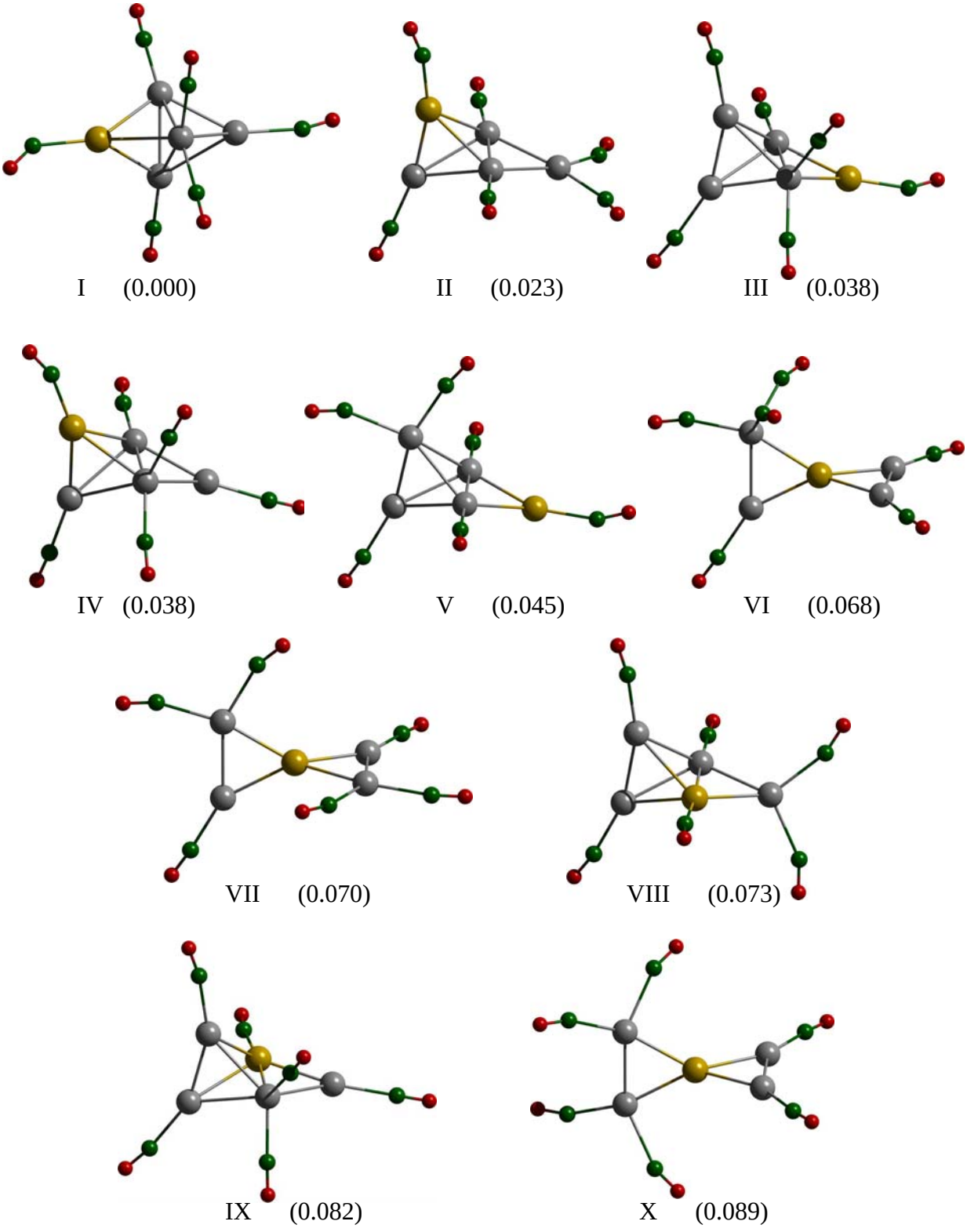


Figure S17: The lowest energy isomers of $Ag_4Au(CO)_6^+$ within 0.1 eV obtained from DFT with B3LYP functional and TZVP atomic basis set.