# Electronic Supplementary Information (ESI)

# Catalytic Activity of Anionic Au-Ag Dimer for Nitric Oxide Oxidation: A DFT Study

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**Table S1:** Binding energies for different binding orientations of $O_2$ and NO with Au-Ag$^-$ dimer

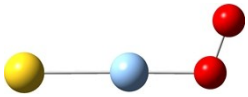
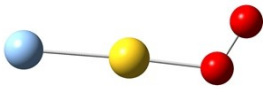
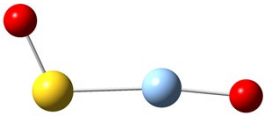
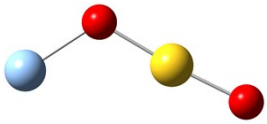
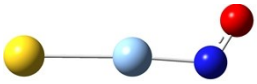
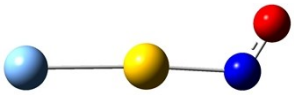
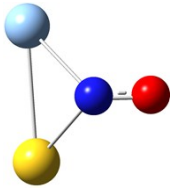
| Structure | Binding Energy (in eV) |
|---|---|
|  | 1.73 |
|  | 1.16 |
|  | 0.03 |
|  | 1.14 |
|  | 0.77 |
|  | 0.56 |
|  | 0.08 |

**Table S2:** Relative energies of different species with various spin multiplicities.

| $AuAg^-$ | | $AuAg^-NO$ | | $AuAg^-O_2$ | |
|---|---|---|---|---|---|
| Multiplicity, S | Relative Energy (in eV) | Multiplicity, S | Relative Energy (in eV) | Multiplicity, S | Relative Energy (in eV) |
| 2 | 0.00 | 1 | 0.00 | 2 | 0.00 |
| 4 | 2.09 | 3 | 0.21 | 4 | 2.35 |
| 6 | 7.91 | | | | |

**Table S3:** Total spin densities of the initial structures

| Species | Total Spin Densities |
|---|---|
| $AuAg^-$ | 1 |
| $Au\text{-}Ag^-O_2$ | 1 |
| $Au\text{-}Ag^-NO$ | 0 |
| $Au\text{-}Ag^-O_2NO$ | 0 |
| $Au\text{-}Ag^-NOO_2$ | 0 |

**Table S4:** Comparison of energies for various species ($E_{(LANL2DZ-LANL2TZ(f))}$) using LANL2DZ and LANL2TZ(f) basis sets on the metal centers.

| Species | $E_{(LANL2DZ-LANL2TZ(f))}$ (in eV) |
|---|---|
| Au-Ag-NO | 0.25 |
| Au-Ag-$NOO_2$ | 0.32 |
| Au-Ag-$NOO_2NO$ | 0.35 |
| Au-Ag-$O_2$ | 0.33 |
| Au-Ag-$O_2NO$ | 0.30 |
| Au-Ag-O | 0.37 |
| Au-Ag-ONO | 0.33 |
| TS1 | 0.32 |
| TS2 | 0.34 |
| TS3 | 0.31 |