SUPPORTING INFORMATION

Photoabsorption of Icosahedral Noble Metal Clusters: an Efficient TDDFT Approach to Large Scale Systems

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Captions to Figures.

Figure S1. Isosurfaces of the imaginary part of the first order time dependent perturbed density calculated at the plasmon energy for $[Ag_{55}]^{3-}$, $[Ag_{147}]^-$ and $[Ag_{309}]^{3+}$. Red and blue surfaces indicate positive and negative isovalue. Isovalue = 0.1.

Figure S2. Isosurfaces of the imaginary part of the first order time dependent perturbed density calculated at energies corresponding to photoabsorption maxima for $[Au_{55}]^{3-}$, $[Au_{147}]^-$ and $[Au_{309}]^{3+}$. Red and blue surfaces indicate positive and negative isovalue. Isovalue = 0.05 for $[Au_{55}]^{3-}$, isovalue = 0.01 for both $[Au_{147}]^-$, and $[Au_{309}]^{3+}$.

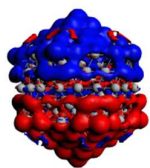**Figure S3.** Photoabsorption profiles of $[Ag_{55}]^{3-}$, $[Ag_{147}]^-$, $[Au_{55}]^{3-}$ and $[Au_{147}]^-$ calculated at TDDFT DZ LB94 level by complex polarizability (black line) and ADF (red line). Imaginary broadening ω_i = 0.15 eV.
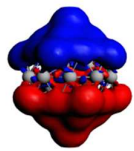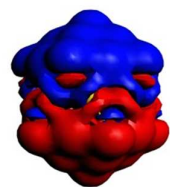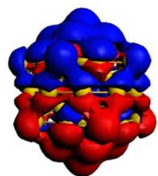
$[Ag_{55}]^{3-}$
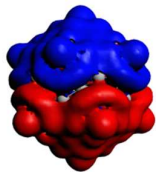
$[Ag_{147}]^{-}$

$[Ag_{309}]^{3+}$

Fig. S1

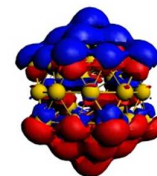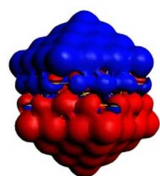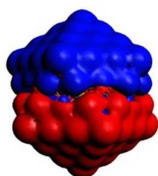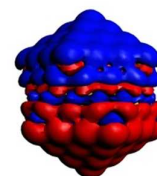$[Au_{55}]^{3-}$ 3.7 eV

$[Au_{55}]^{3-}$ 4.3 eV

$[Au_{55}]^{3-}$ 5.4 eV
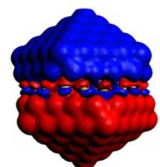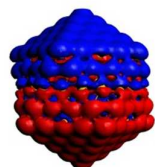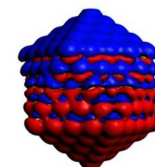
$[Au_{147}]^{-}$ 3.5 eV

$[Au_{147}]^{-}$ 4.1 eV

$[Au_{147}]^{-}$ 5.5 eV

$[Au_{309}]^{3+}$ 3.5 eV

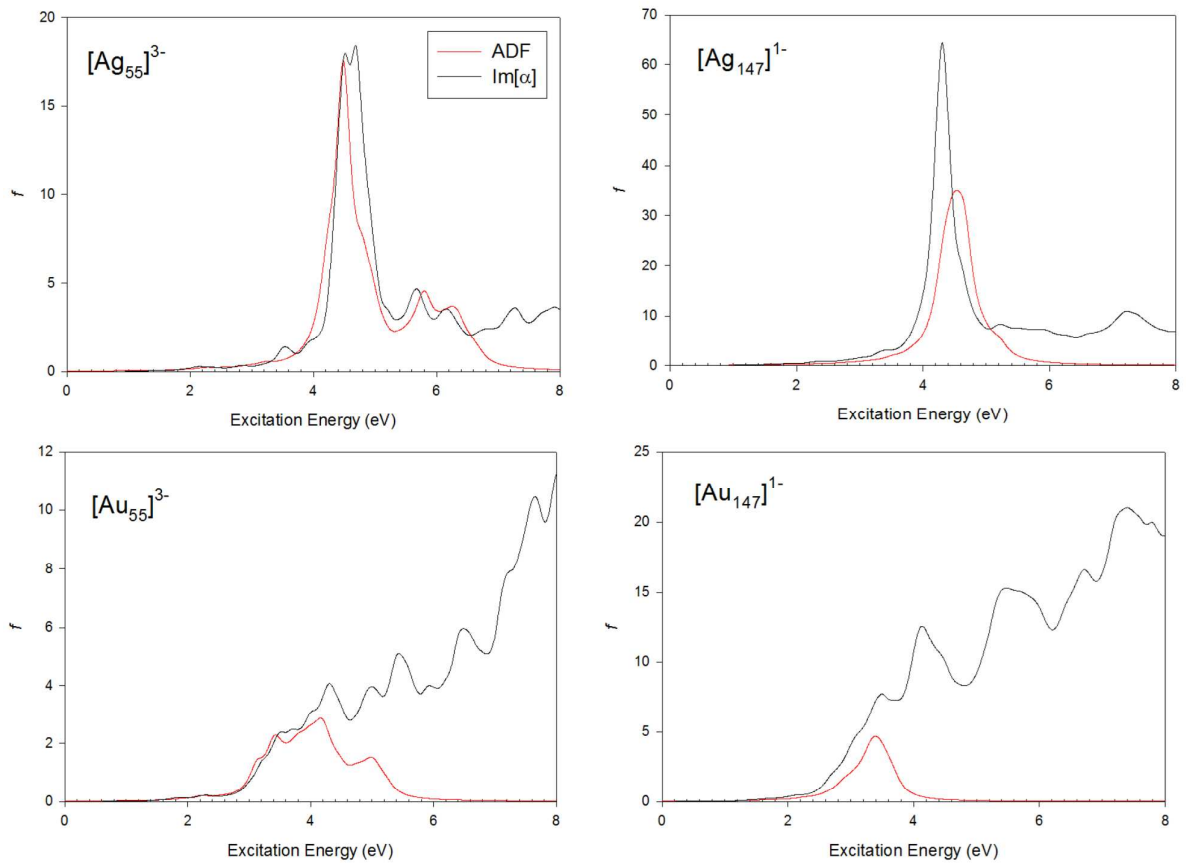$[Au_{309}]^{3+}$ 4.4 eV

$[Au_{309}]^{3+}$ 5.5 eV

Fig. S2

Fig. S3