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# Theoretical Study of the Stability, Structure, and Optical Spectra of Small Silver Clusters and Their Formation Using Density Functional Theory

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**Supporting Information**

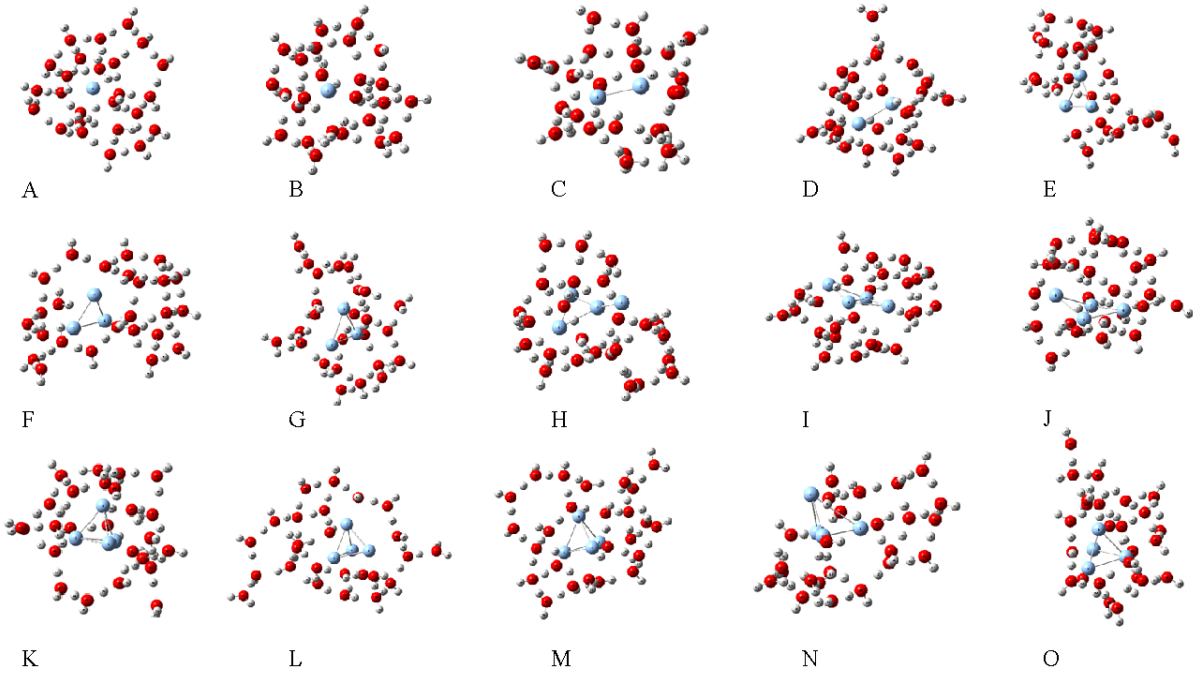


Figure S1. Optimized structures of initial (A) Ag, (B) $Ag^{+}$, (C) $Ag_2$, (D) $Ag_2^{+}$, (E) $Ag_3$, (F) $Ag_3^{+}$, (G) $Ag_3^{2+}$, (H) $Ag_4$ planar, (I) $Ag_4$ tetrahedral, (J) $Ag_4^{+}$ planar, (K) $Ag_4^{+}$ tetrahedral, (L) $Ag_4^{2+}$ planar, (M) $Ag_4^{2+}$ tetrahedral, (N) $Ag_4^{3+}$ planar, and (O) $Ag_4^{3+}$ tetrahedral configurations with 25 explicit water molecules around each species using BP86/LANL2DZ level of theory in Gaussian 16 software. Ag, O, and H atoms are represented using light blue, red, and grey colors respectively.

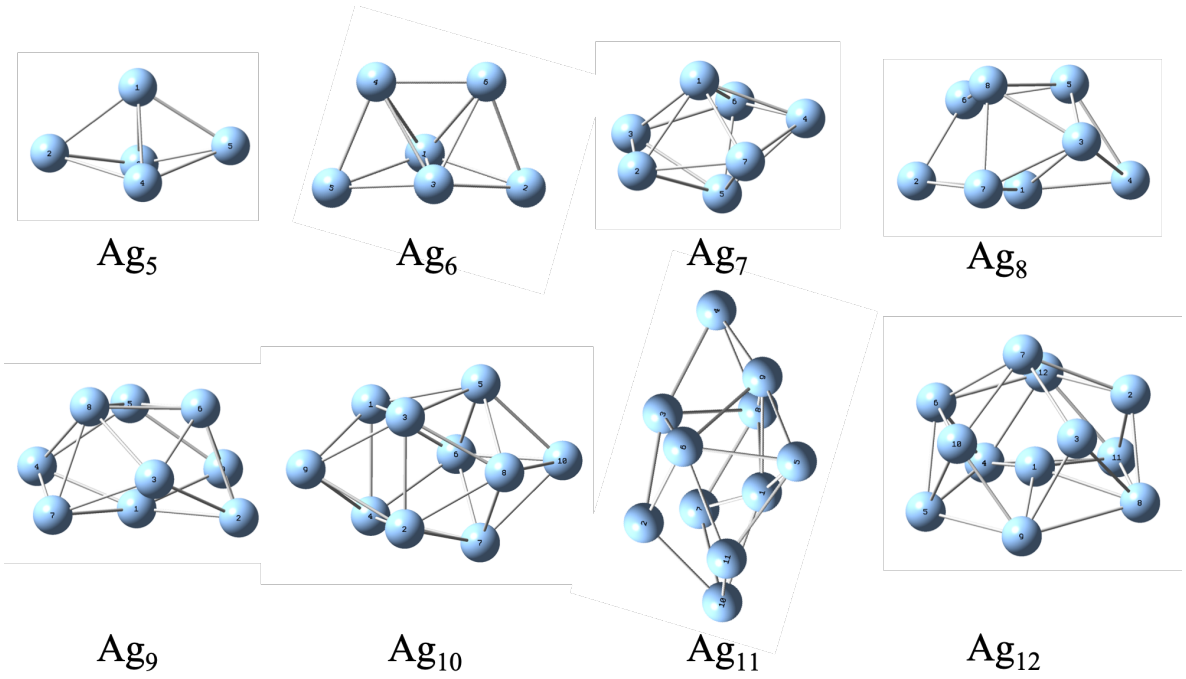


Figure S2. Optimized structures of $Ag_5$ to $Ag_{12}$ in gas phase using BP86/LANL2DZ level of theory in Gaussian 16 software.

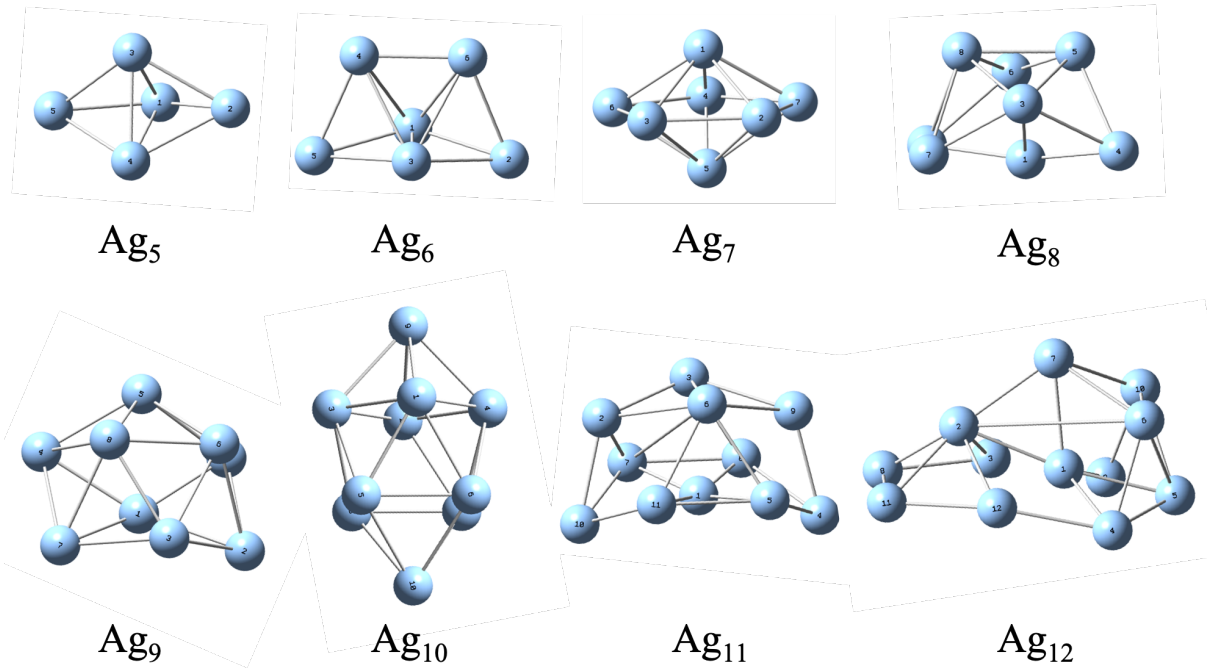


Figure S3. Optimized structures of $Ag_5$ to $Ag_{12}$ in implicit aqueous solution using BP86/LANL2DZ level of theory in Gaussian 16 software.

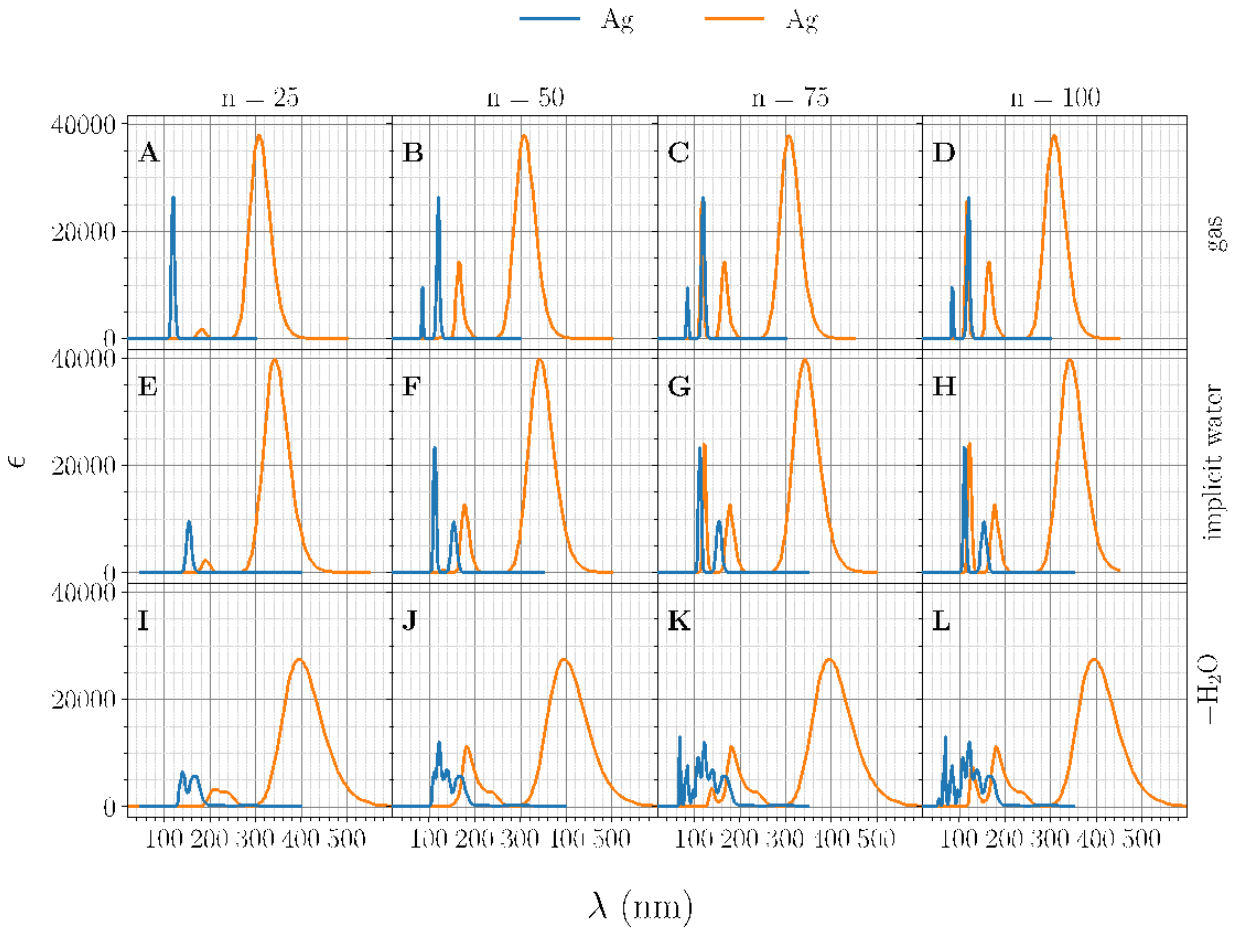


Figure S4. Absorption spectra of $Ag^+$ and Ag with 25, 50, 75, and 100 excited electronic states in gas phase (A-D) in aqueous phase (E-H), and spectra of $AgH2O^+$ and AgH2O (I-J) using TDDFT at the BP86/LANL2DZ level of theory.

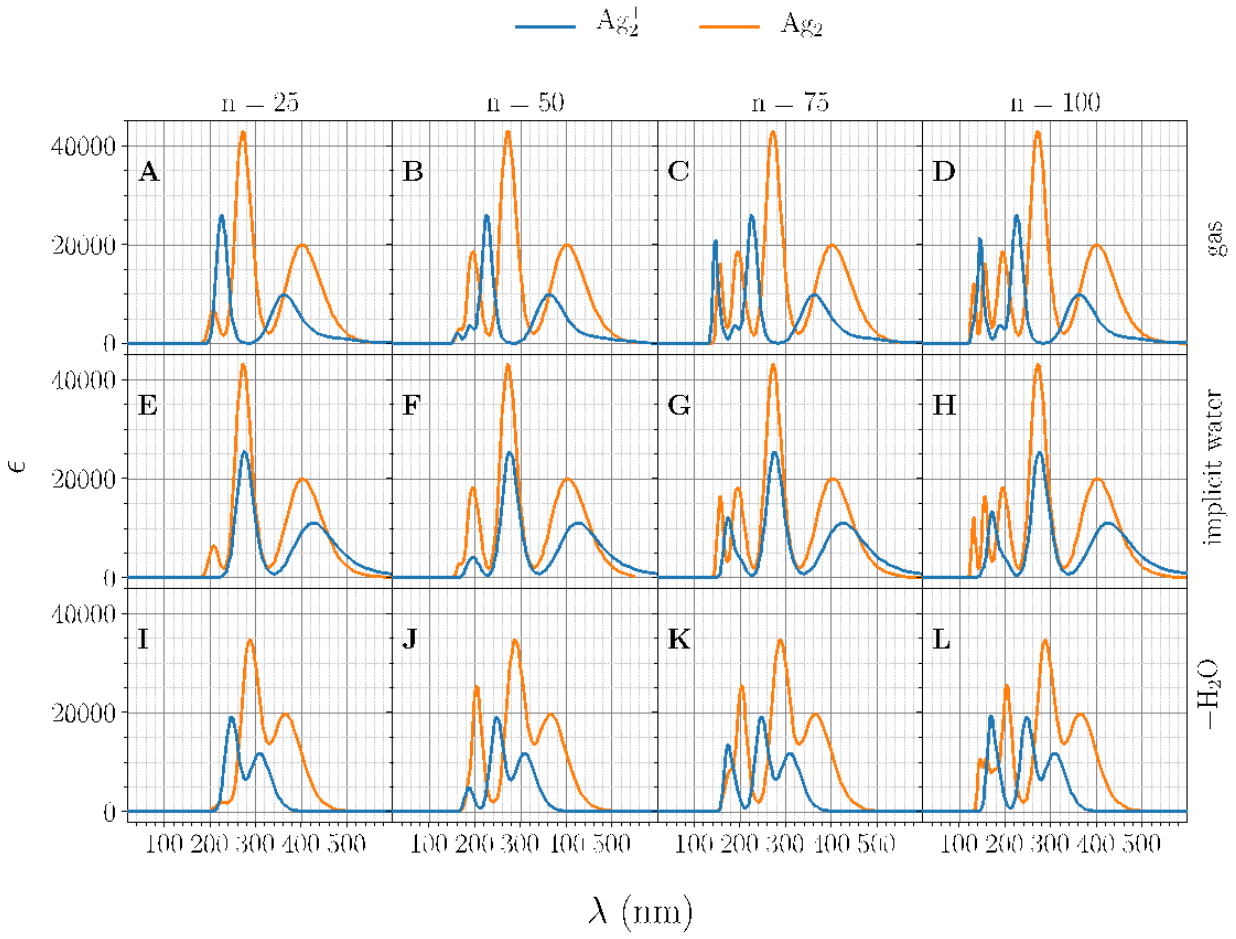


Figure S5. Absorption spectra of $Ag_2^+$ and $Ag_2$ with 25, 50, 75, and 100 excited electronic states in gas phase (A-D) in aqueous phase (E-H), and spectra of $Ag_2(H_2O)_2^+$ and $Ag_2(H_2O)_2$ (I-J) using TDDFT at the BP86/LANL2DZ level of theory.

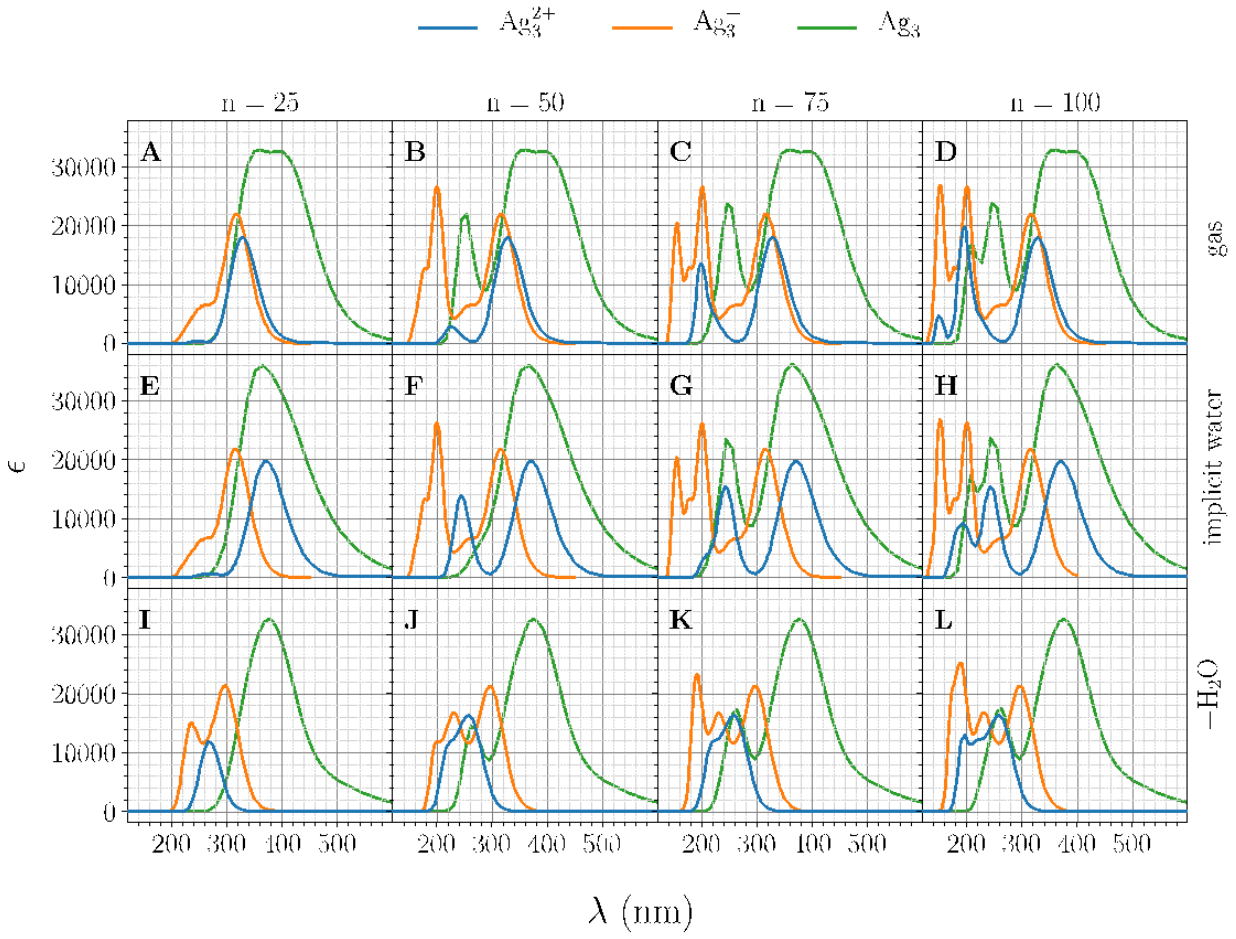


Figure S6. Absorption spectra of $Ag_3^{2+}$, $Ag_3^+$, and $Ag_3$ with 25, 50, 75, and 100 excited electronic states in gas phase (A-D) in aqueous phase (E-H), and spectra of $Ag_3(H_2O)_3^+$ and $Ag_3(H_2O)_3$ (I-J) using TDDFT at the BP86/LANL2DZ level of theory.

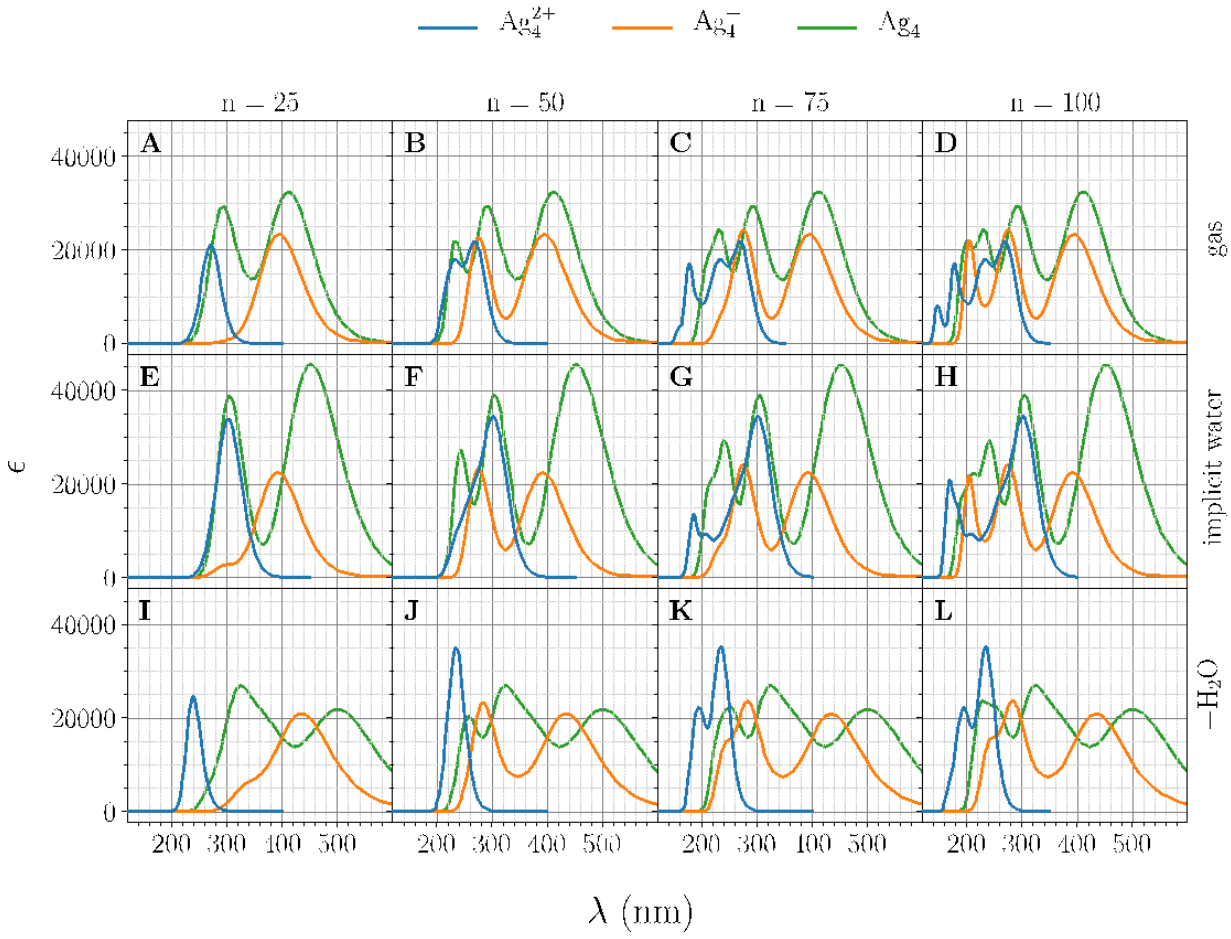


Figure S7. Absorption spectra of $Ag_4^{2+}$, $Ag_4^+$, and $Ag_4$ with 25, 50, 75, and 100 excited electronic states in gas phase (A-D) in aqueous phase (E-H), and spectra of $Ag_4(H_2O)_4^+$ and $Ag_4(H_2O)_4$ (I-J) using TDDFT at the BP86/LANL2DZ level of theory.