Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Interfacial charge transfer complex formation between silver nanoparticles and aromatic amino acids

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Figure S1. The calculated electronic excitation spectra of amino acids (Trp, His, and Ala).

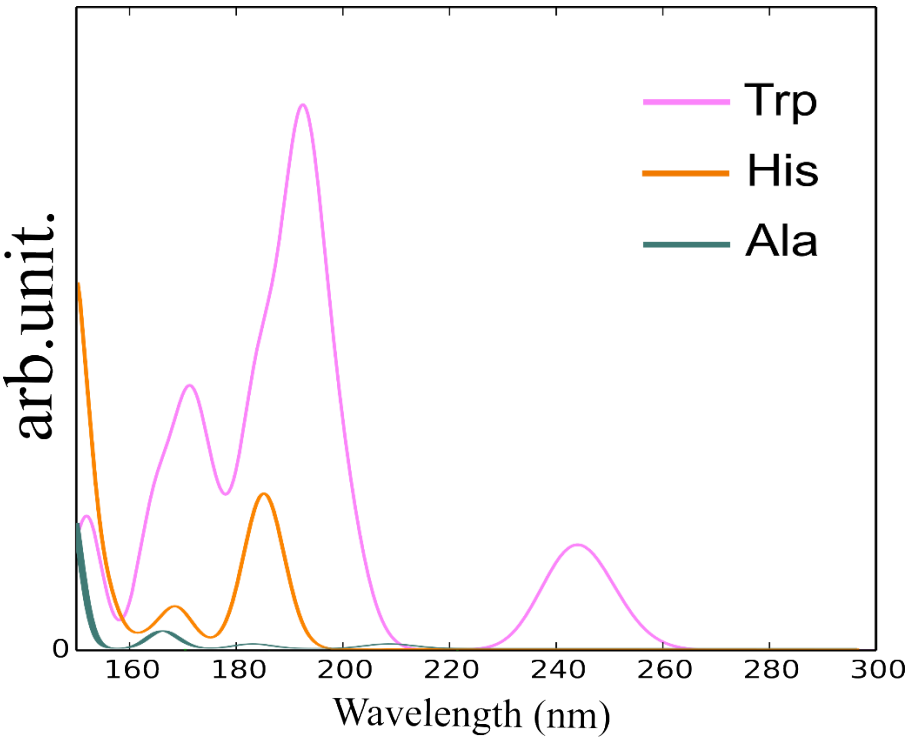

Figure S2. The relevant orbitals involved in selected electron transitions for Trp/Ag_{19} cluster.

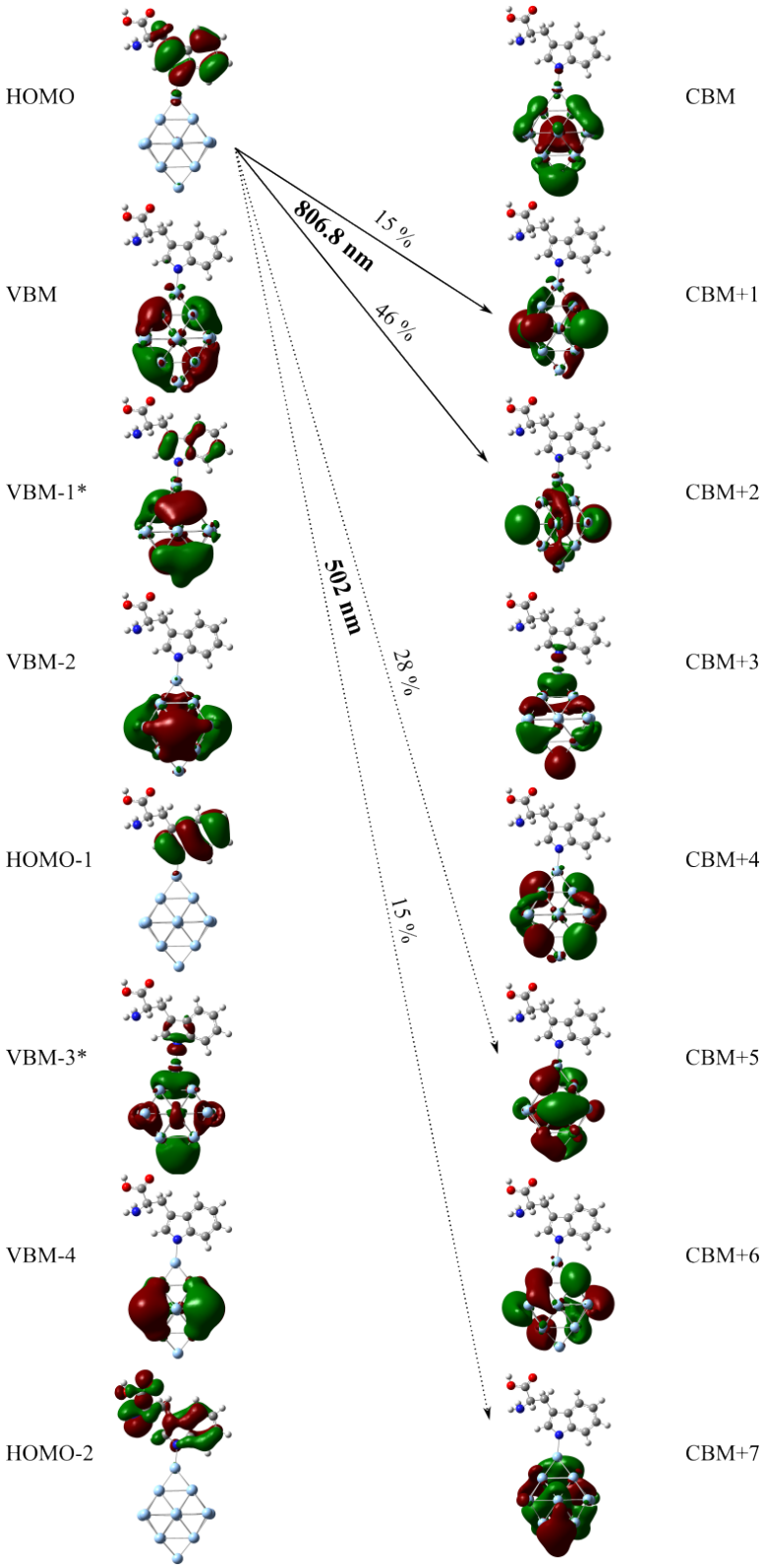

Figure S3. The relevant orbitals involved in selected electron transitions for His/Ag_{19} cluster.

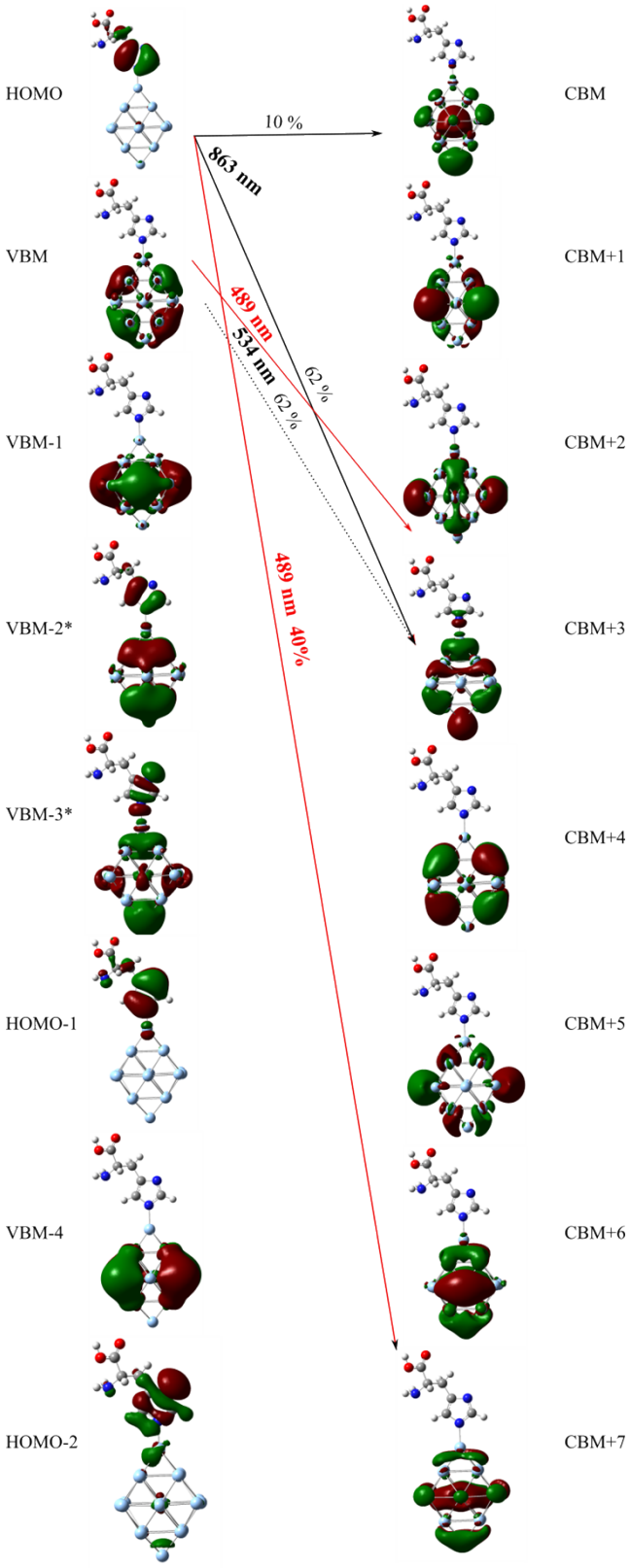

Figure S4. The relevant orbitals involved in selected electron transitions for Ala/Ag_{19} cluster.

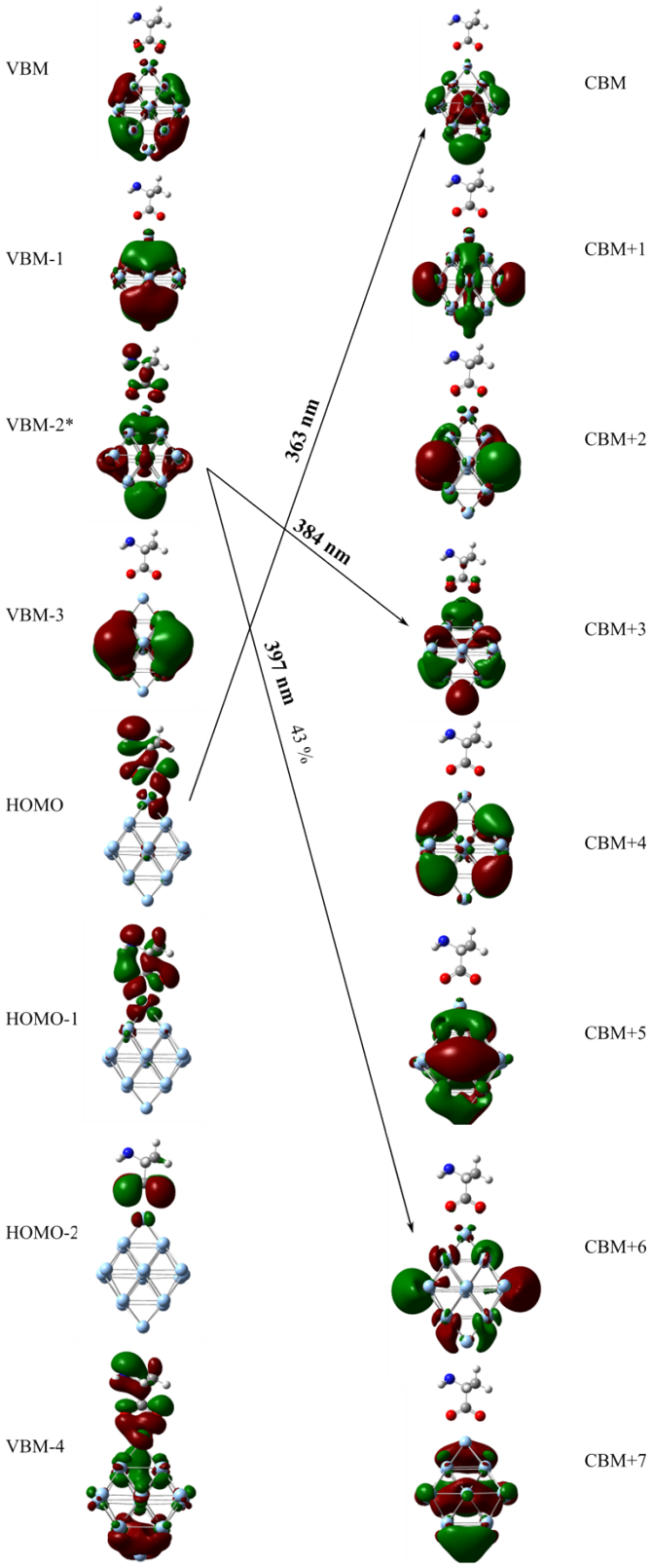

Figure S5. Total and partial densities of states (DOS/PDOS) and spatial electron distributions of selected orbitals of **(A)** H/Ag_{19} cluster and **(B)** Ala/Ag_{19} complex as calculated at CAM-B3LYP/*def2*-SVP level. Gray: carbon, white: hydrogen, blue: nitrogen, red: oxygen, bluish: silver atoms.

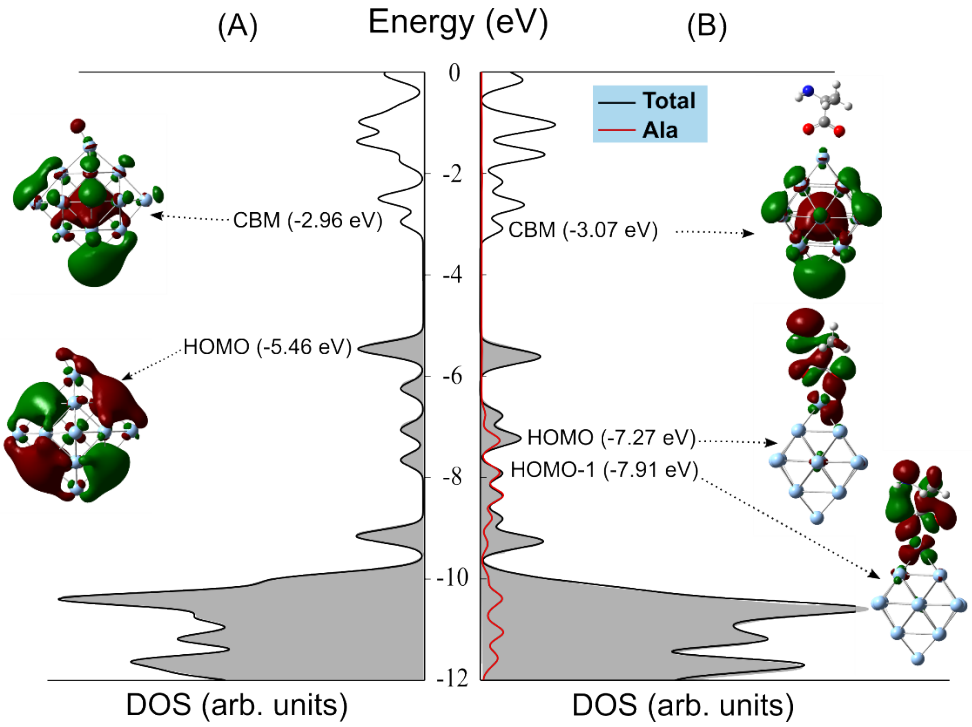

Figure S6. Typical TEM image of unmodified Ag NPs.

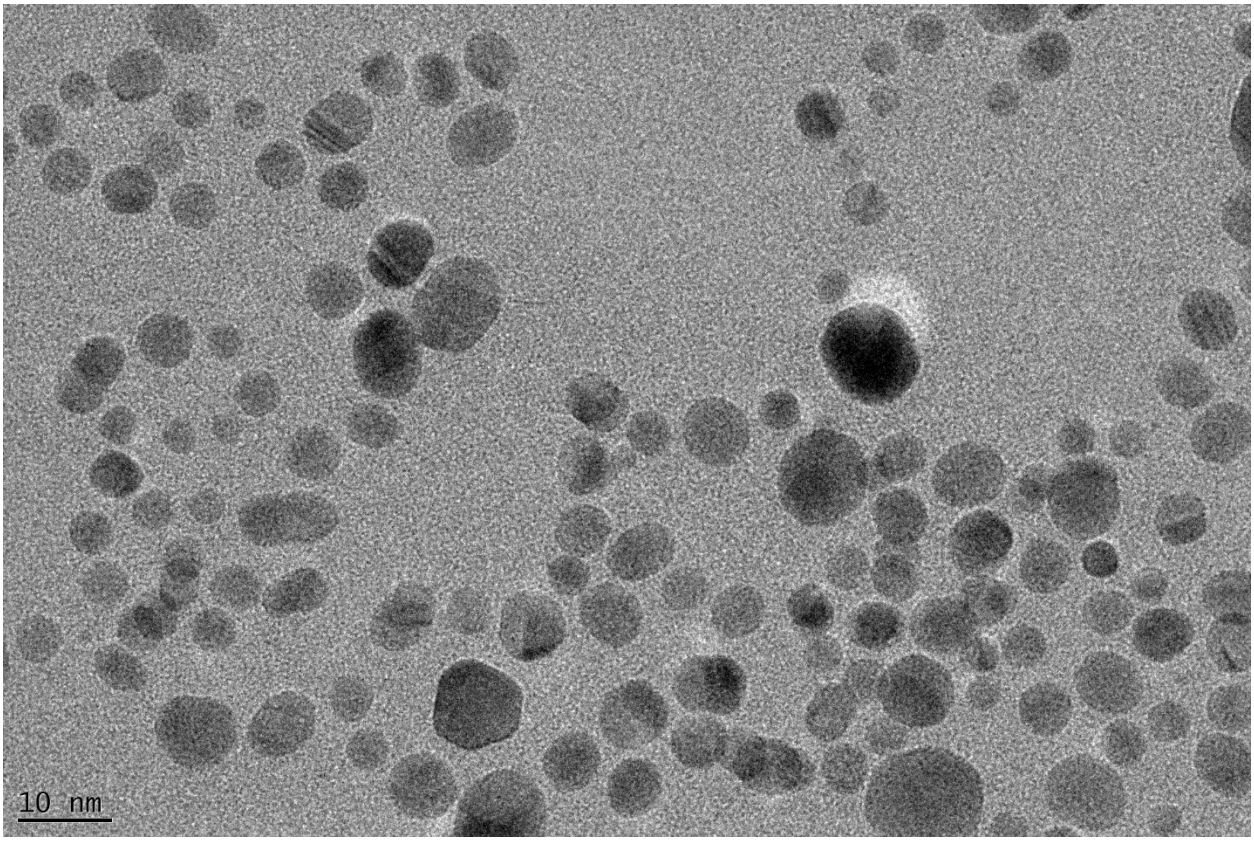

Figure S7. The time-dependent absorption spectra of His/Ag colloid; concentrations: 1×10^{-4} M Ag and 4.0 mM His.

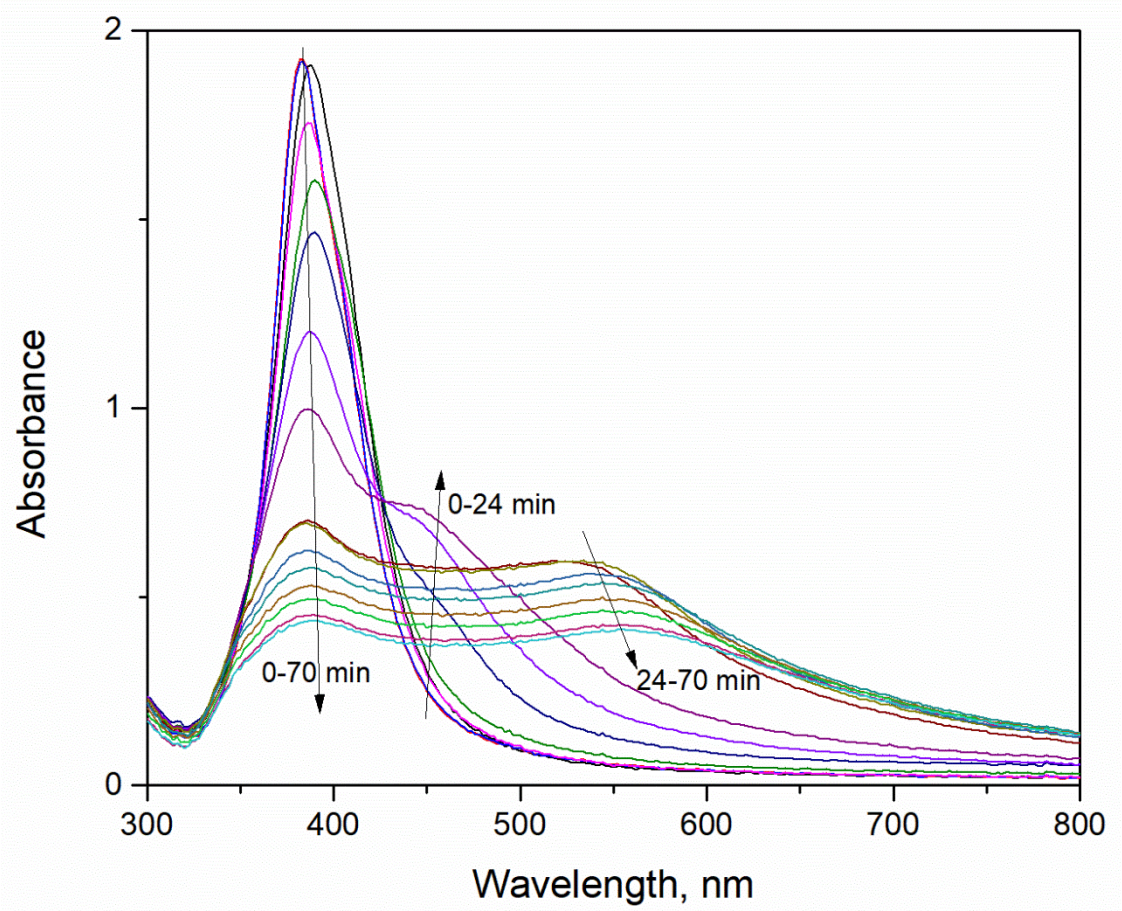

Figure S8. The time-dependent absorption spectra of Ala/Ag colloid (concentrations: 1×10^{-4} M Ag and 4.0 mM Ala); inset: absorbance of pristine Ag colloid at 388 nm as a function of time.