

Supplementary Information: Strong-field effects in the photo-induced dissociation of the hydrogen molecule on a silver nanoshell

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1 Additional figures

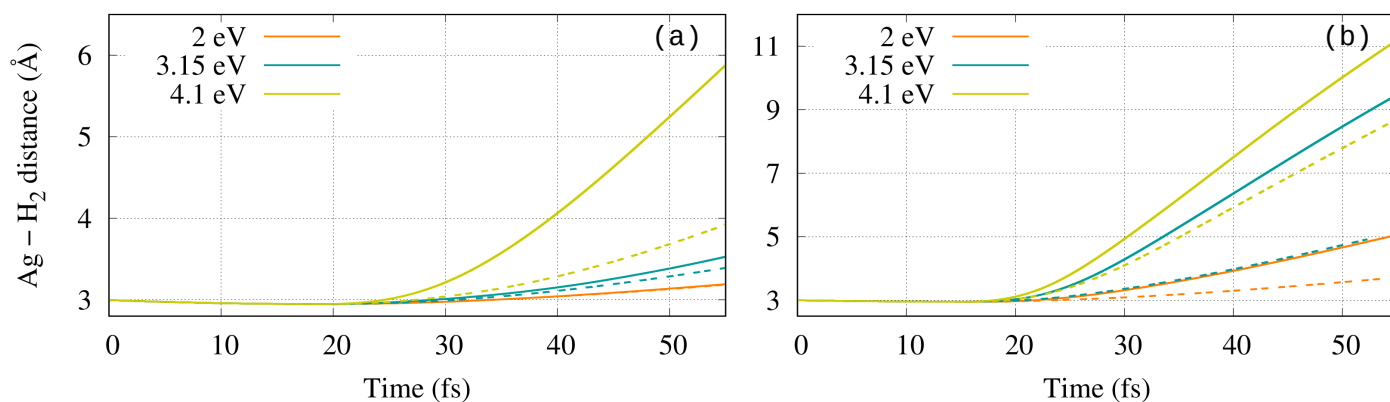


Figure S1 Distance from the top Ag atom to the center of the H₂ molecule as a function of time: (a) $I_{\max} = 2 \times 10^{13}$ W/cm², (b) $I_{\max} = 1 \times 10^{14}$ W/cm². Solid (dashed) lines correspond to the calculations with (without) ghost atoms.

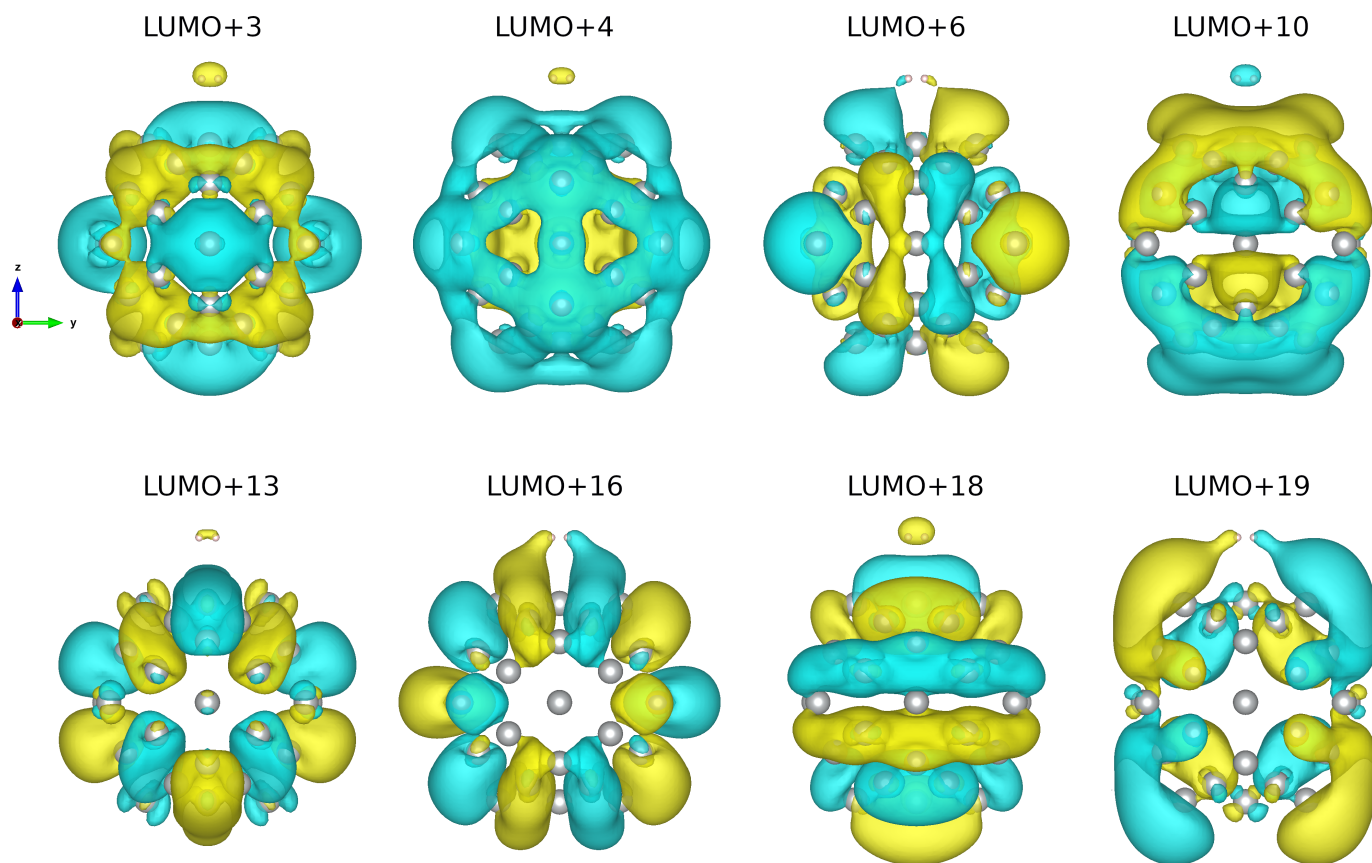


Figure S2 Ground-state unoccupied molecular orbitals of $\text{Ag}_{55}^{\text{L1}} + \text{H}_2$. Orbitals LUMO+3, +4, +10, +13, and +18 have a bonding, while LUMO+6, +16, and +19 have an antibonding character on H_2 .

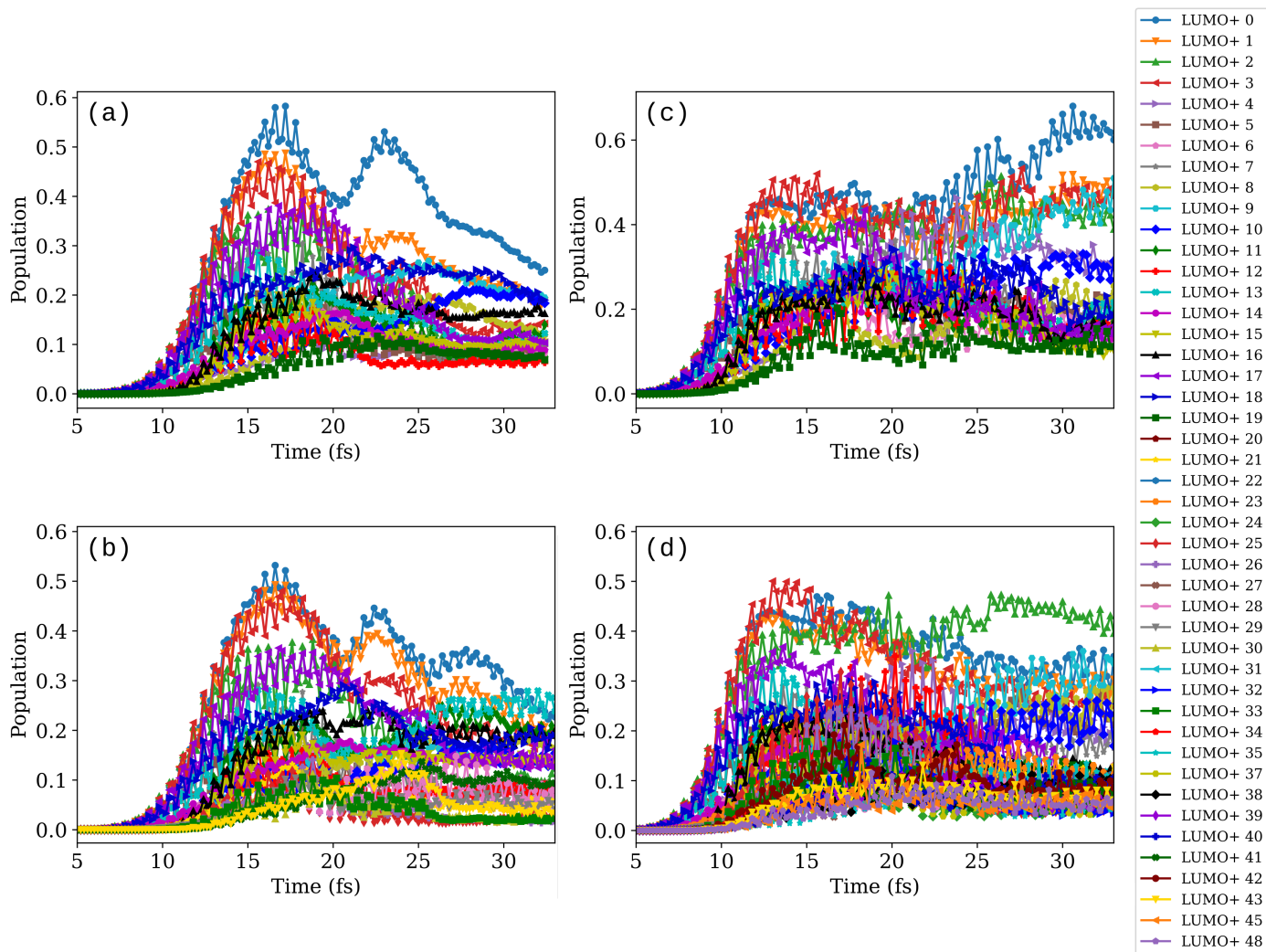


Figure S3 Time evolution of the $\text{Ag}_{55}^{\text{L1}}+\text{H}_2$ orbital populations induced by an external field with intensity (left panels, (a,b)) $I_{\text{max}} = 2 \times 10^{13} \text{ W/cm}^2$ and (right panels, (c,d)) $I_{\text{max}} = 1 \times 10^{14} \text{ W/cm}^2$. (a) and (c) correspond to the case without the ghost atoms, while (b) and (d) - with the ghost atoms. The field frequency is $\hbar\omega_0 = 3.15 \text{ eV}$. Orbital populations are calculated every 0.2 fs as sums of the squares of the projections of the time-dependent occupied MOs on the initially unoccupied orbitals. Only populations with maximum values > 0.1 are plotted.

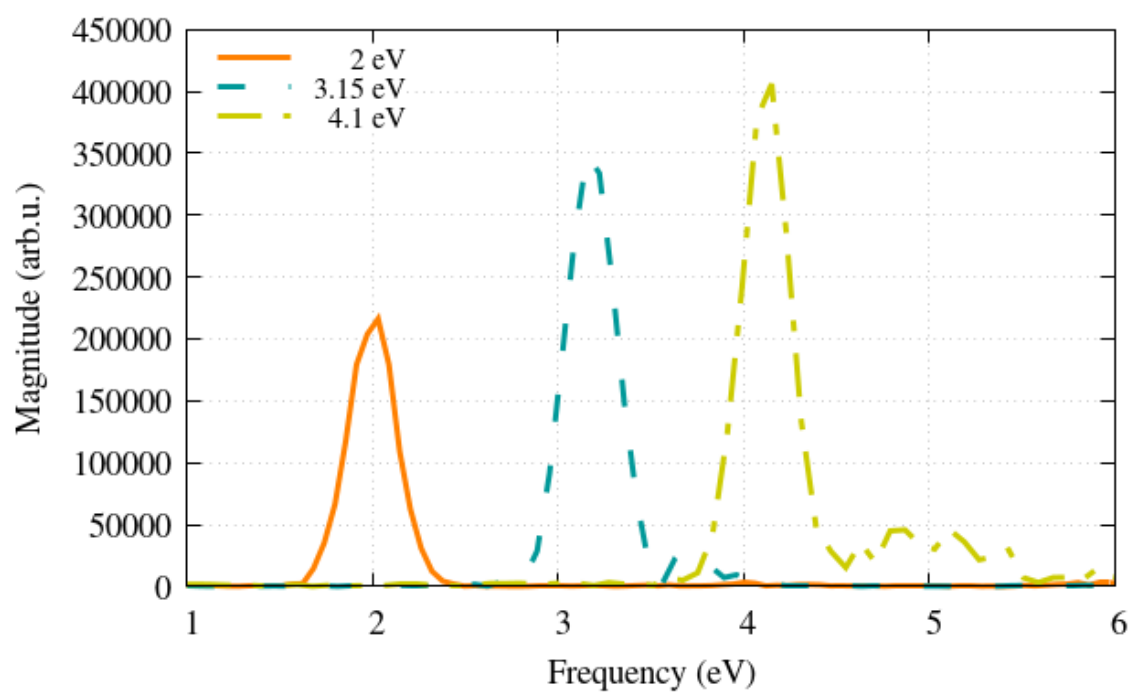


Figure S4 Fourier transform of the time-dependent dipole moment at field intensity $I_{\max} = 2 \times 10^{13} \text{ W/cm}^2$.

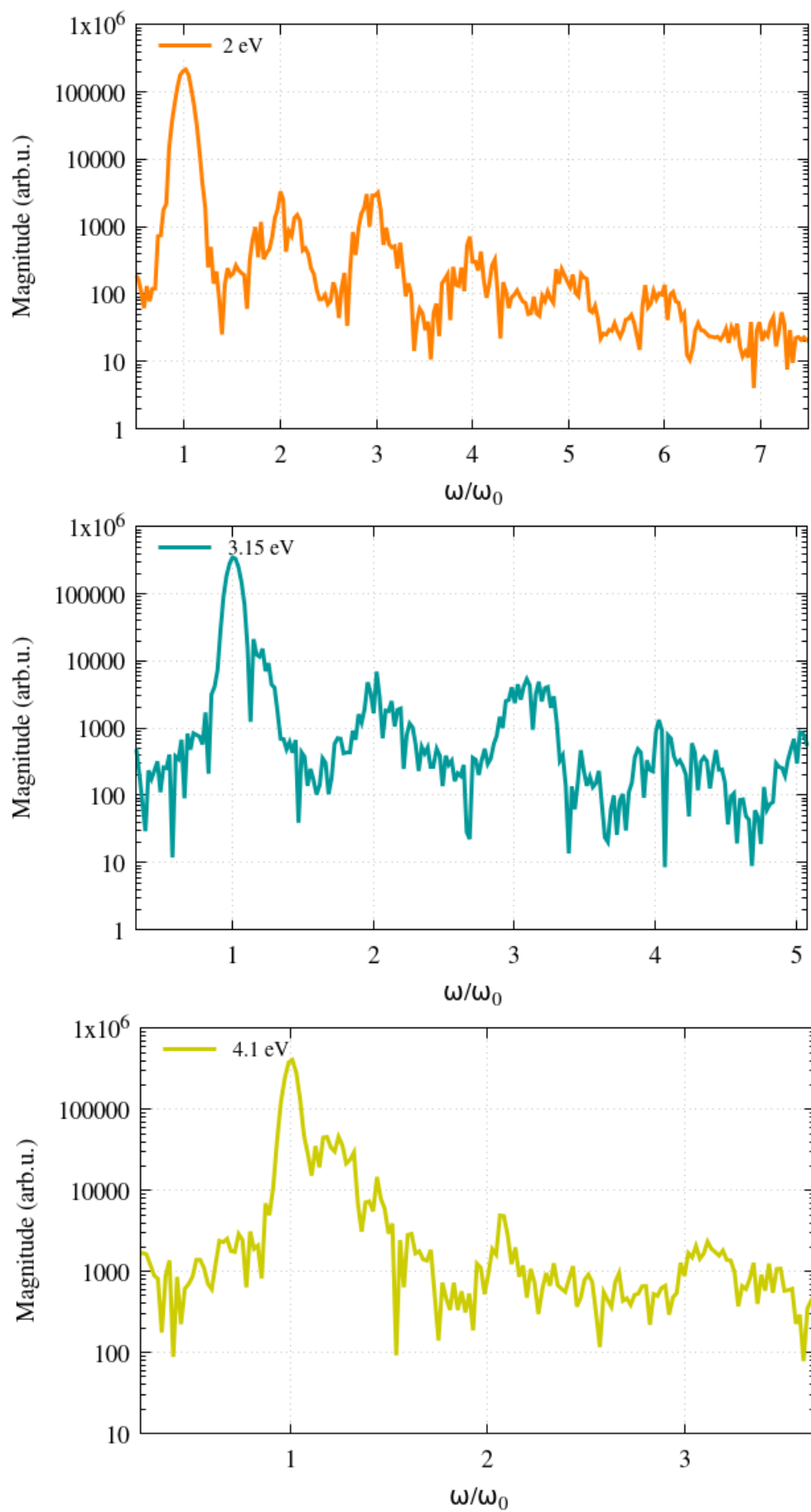


Figure S5 Fourier transform of the time-dependent dipole moment at field intensity $I_{\max} = 2 \times 10^{13}$ W/cm² and frequencies (a) 2 eV, (b) 3.15 eV, (c) 4.1 eV. Higher harmonics are observed on a logarithmic scale.

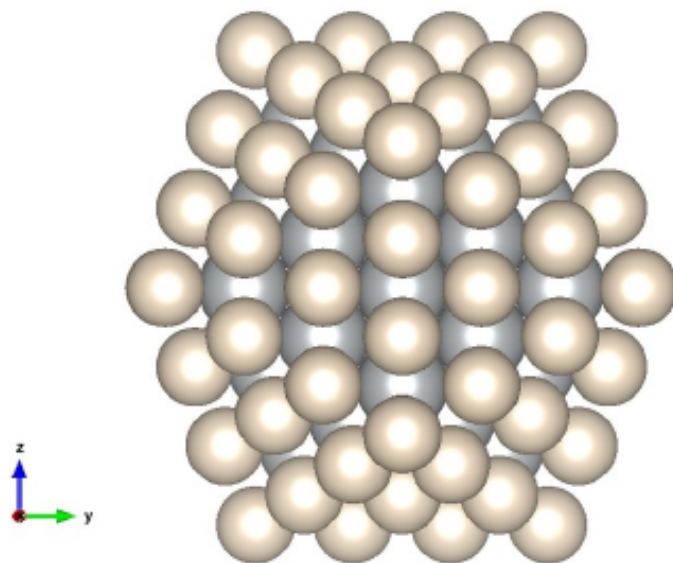


Figure S6 Atomic structure of the $\text{Ag}_{55}^{L1} + \text{H}_2$ surrounded by the layer of ghost atoms Ag_g . Ag atoms in grey and Ag ghost atoms in white.

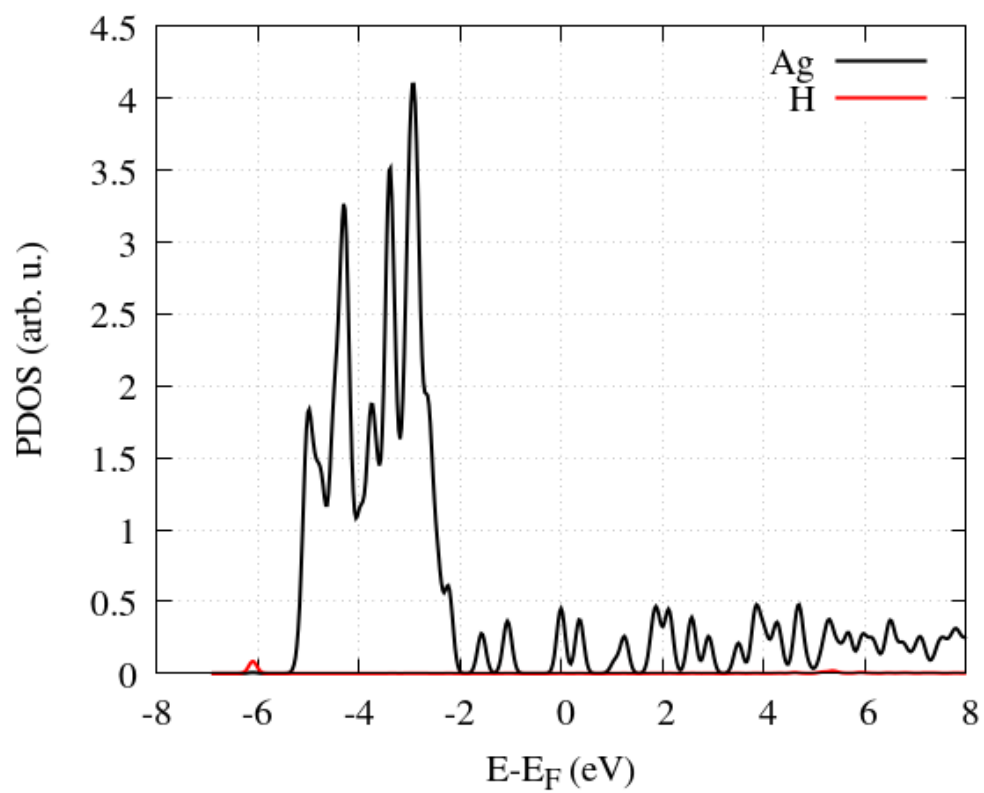


Figure S7 PDOS of the $\text{Ag}_{55}^{L1} + \text{H}_2$.

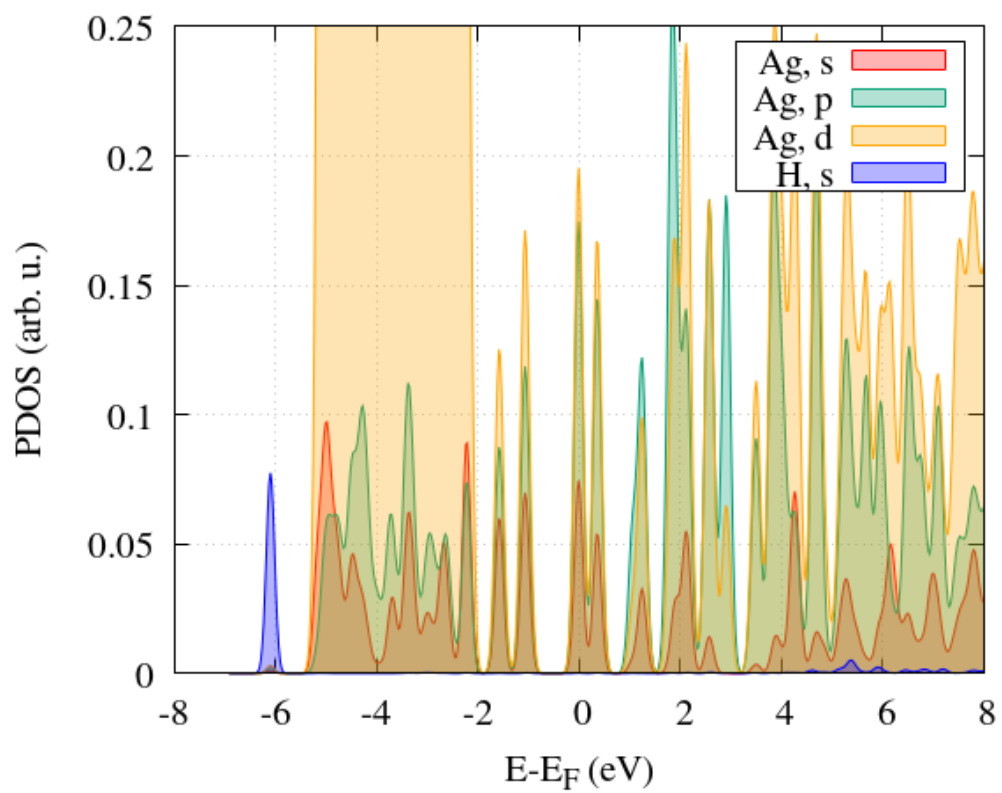


Figure S8 Angular-momentum resolved PDOS of the $\text{Ag}_{55}^{L1} + \text{H}_2$. The vertical axis scale is reduced to show the small features.

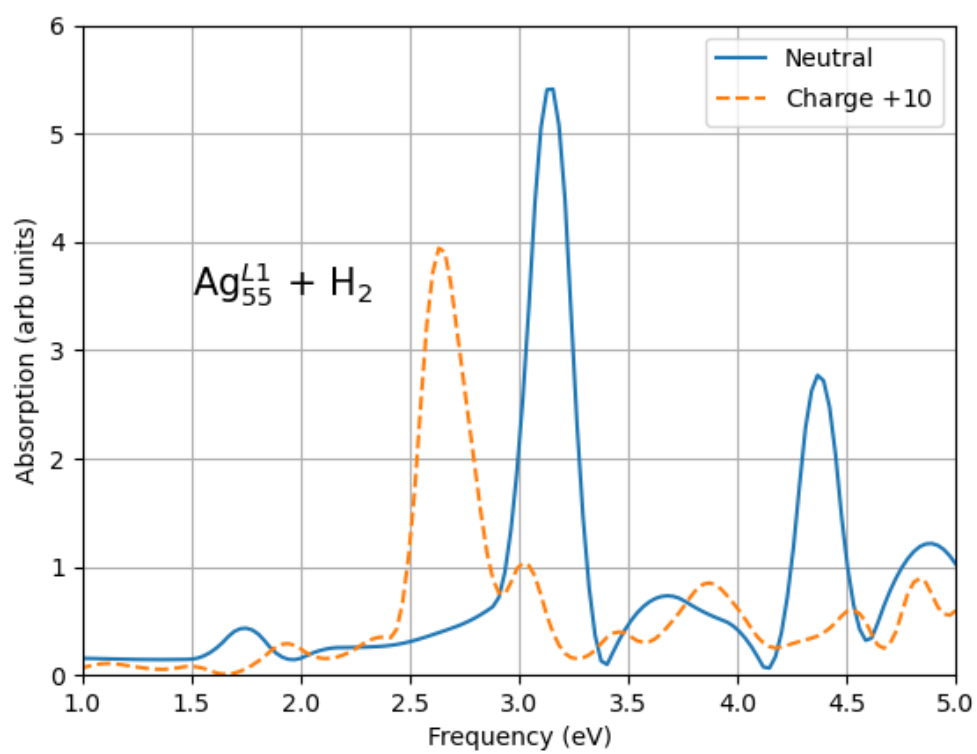


Figure S9 Absorption spectrum for neutral and charged system $\text{Ag}_{55}^{\text{L1}} + \text{H}_2$.