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

Understanding the Mechanism of Plasmon-Driven Water Splitting: Hot Electron Injection and Near Field Enhancement Effect

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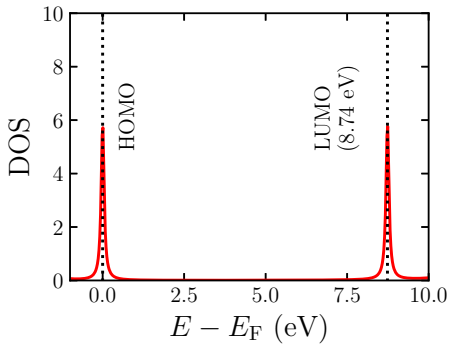

Figure S1: The DOS of the isolated H_2O molecule (HOMO energy is set to zero)

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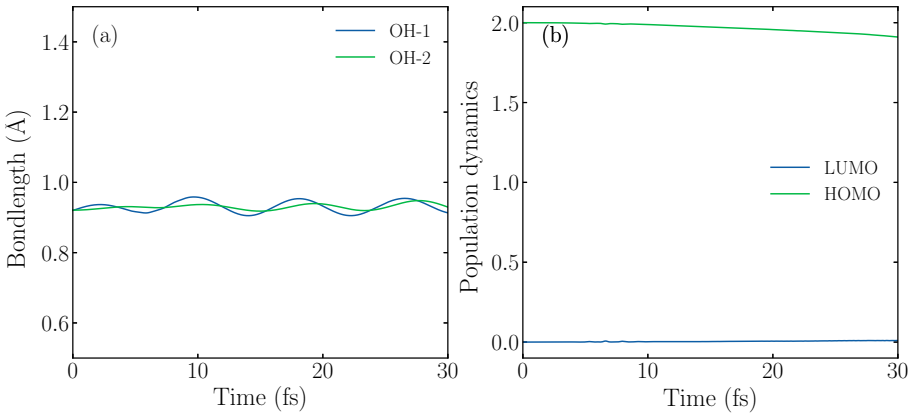

Figure S2: (a) The time evolution of OH bond when an isolated H_2O molecule interacts with the laser field with E_{max} =1.80 V/Å and ω =3.07 eV, respectively. (b) The electrons population dynamics on HOMO and LUMO of the isolated H_2O molecule. The optimized OH bond lengths of H_2O in the ground state are 0.92 Å.

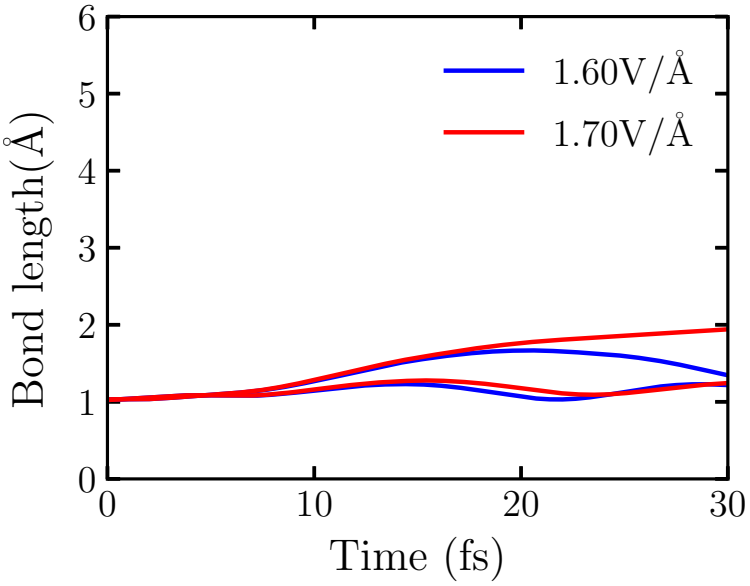

Figure S3: Time evolution of OH bonds in Au_{20}@H_2O system under the laser field with E_{max} =1.60 V/Å and E_{max} =1.70 V/Å, respectively.

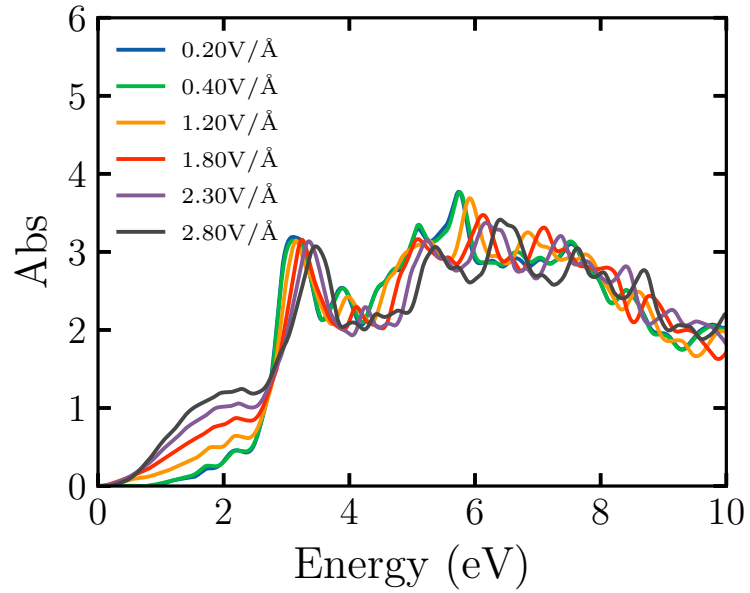

Figure S4: The absorption spectra of Au_{20}@H_2O vary with the laser field strength. We note that the incident laser field is polarized along the $+z$ direction. $\vec{E}_0(t) = \vec{E}^0_{max} e^{-(t-t_0)^2/2\tau^2}$, where t_0 =0.00 fs and τ =0.01 fs, is assumed.

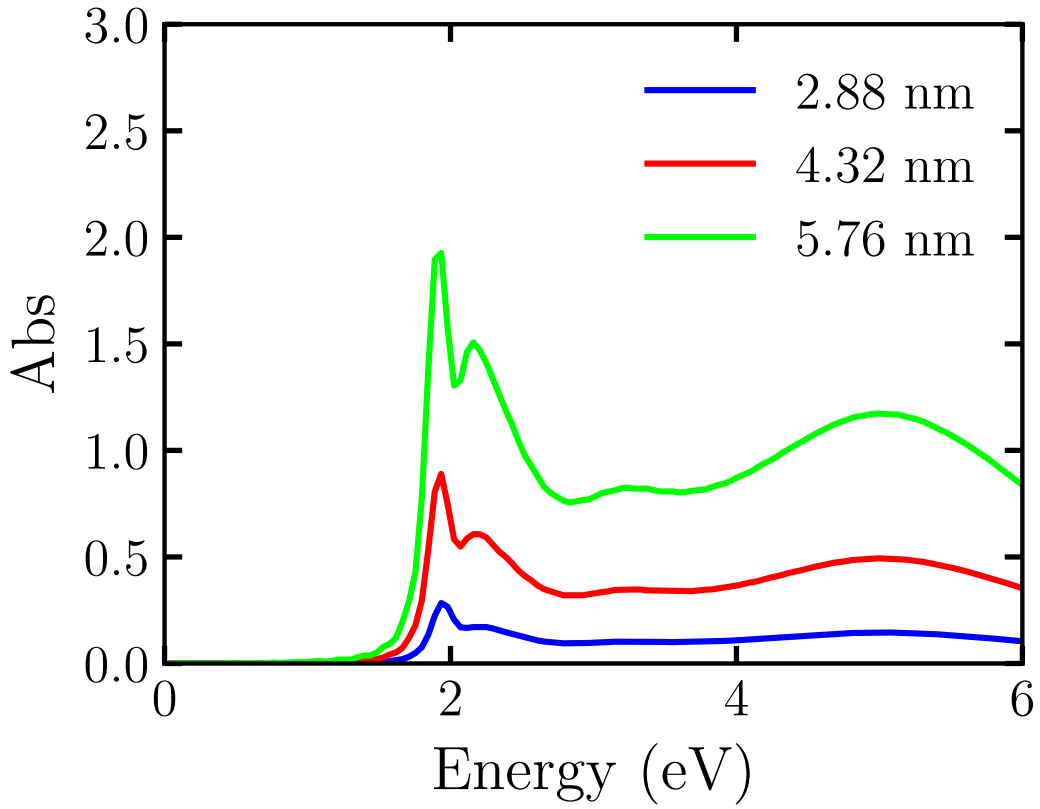

Figure S5: The absorption spectra of Au tetrahedrons with the side length of L=2.88 nm, 4.32 nm, and 5.76 nm calculated by FDTD.

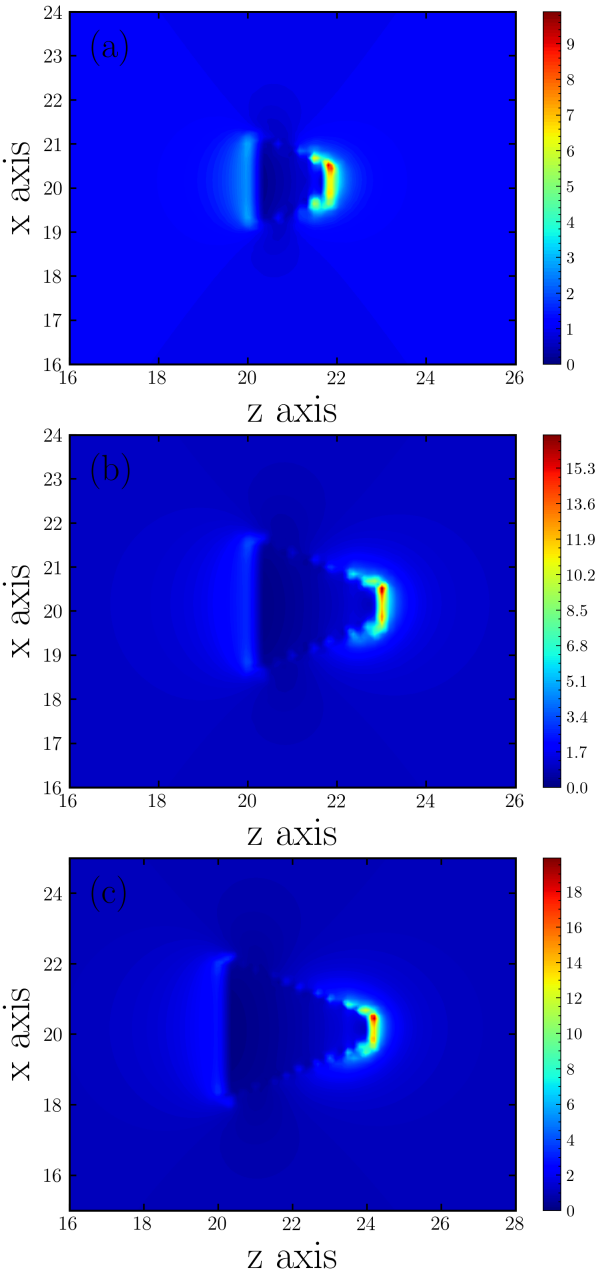

Figure S6: The contour plot (XZ plane) of the electric field enhancement $|E(\omega)|^2/|E_0(\omega)|^2$ (ω corresponding to the absorption peak 3.07 eV) of a Au tetrahedron with side length (a) 2.88 nm; (b) 4.32 nm; (c) 5.76 nm.

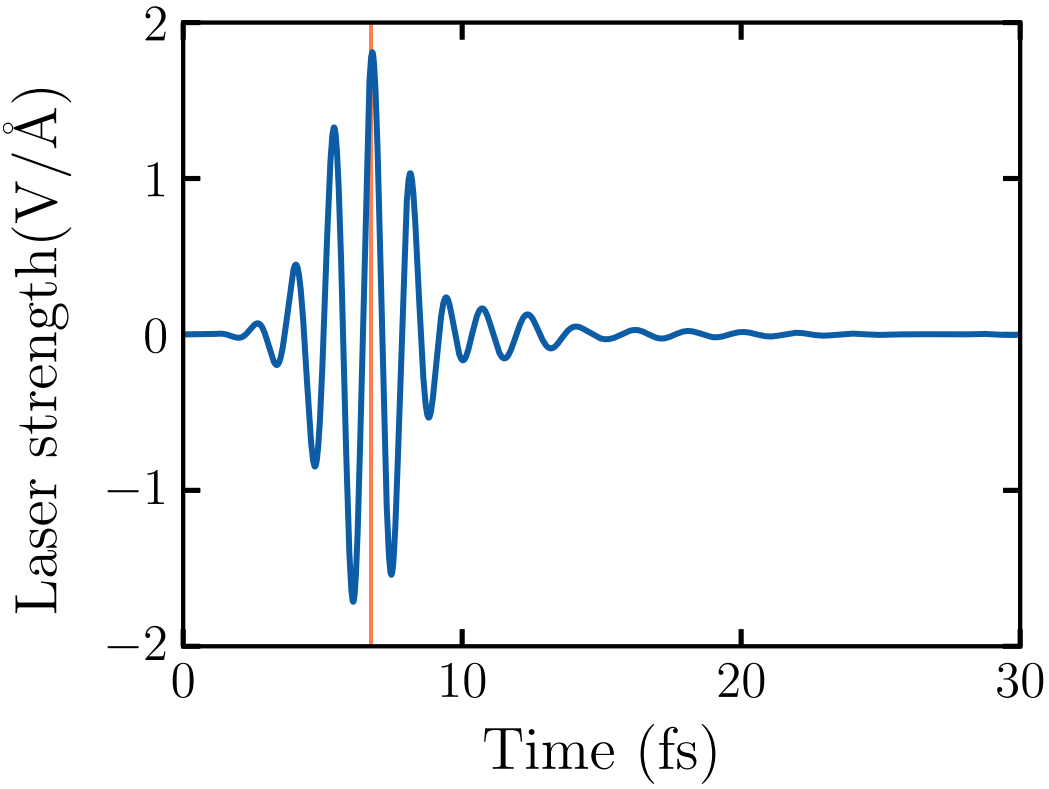

Figure S7: The scattered field in $+z$ direction for the observed point which is set at the center of mass of Au_{20}@H_2O. And the forces act on H_2O in 'coral' color area are plotted in Figure S8.

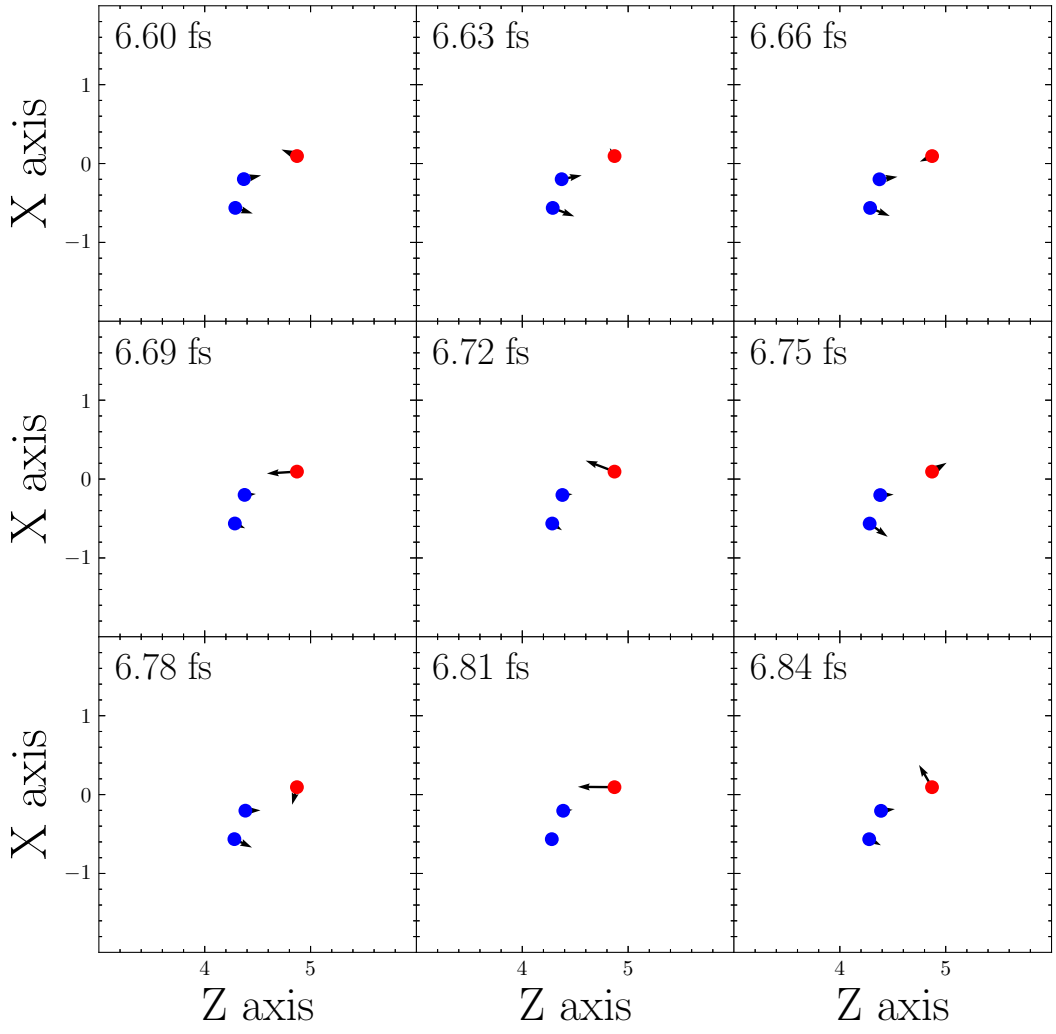

Figure S8: The force acted on H_2O molecule in the XZ plane under a uniform field, the blue dots mean H atoms and red one means O atom.

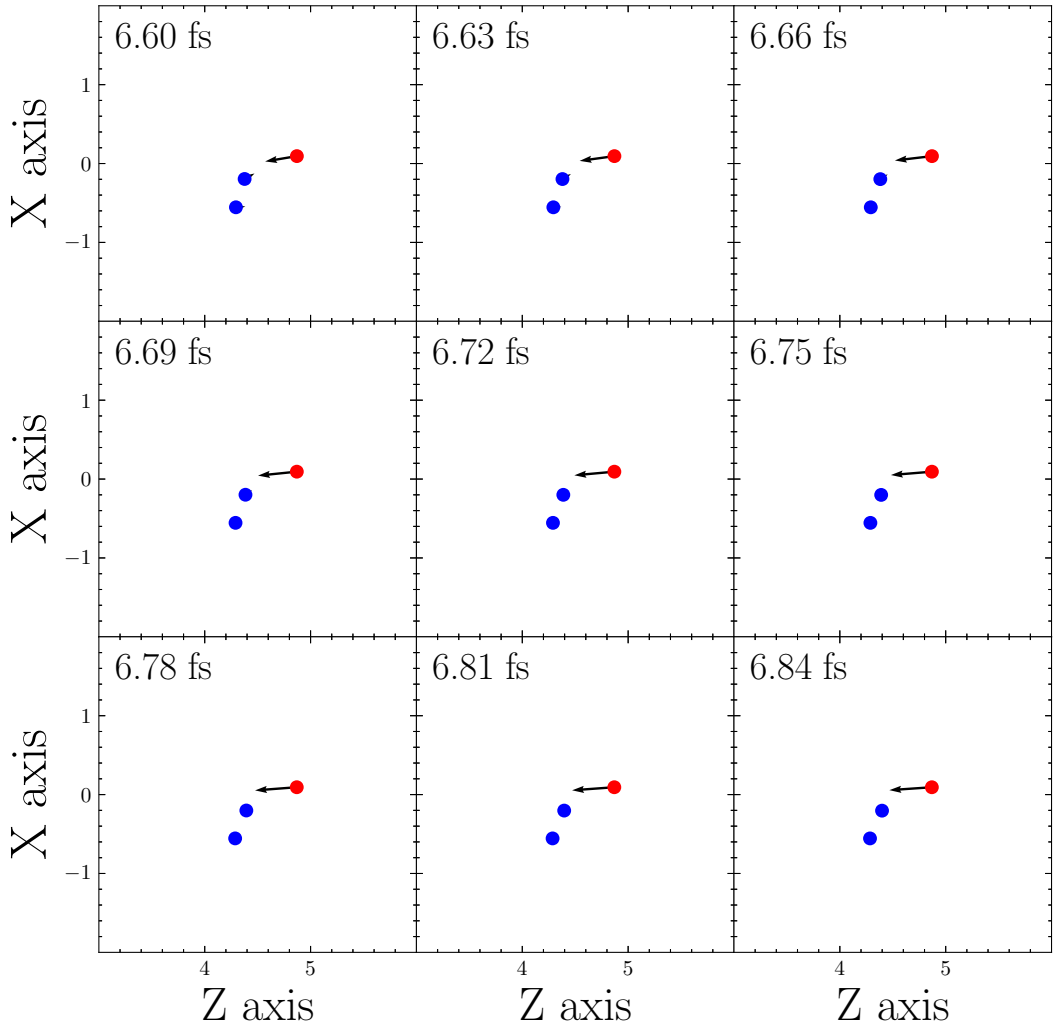

Figure S9: The force acted on H_2O molecule in the XZ plane under the near field, the blue dots mean H atoms and red one mean O atom.