Supplementary information for:
Ab initio insights into plasmonic and strong-field contributions to H_2 dissociation on silver nanoshells

Natalia E. Koval,*[a] J. Iñaki Juaristi,[b,a,c] and Maite Alducin*[a,c]

[a] *Centro de Física de Materiales CFM/MPC (CSIC-EHU), Paseo Manuel de Lardizabal 5, 20018 Donostia-San Sebastián, Spain; E-mail: natalia.koval@ehu.eus*

[b] *Departamento de Polímeros y Materiales Avanzados: Física, Química y Tecnología, Facultad de Química (EHU), Apartado 1072, 20080 Donostia-San Sebastián, Spain*

[c] *Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain*

S1 Gaussian pulses used in TDDFT-ED simulations

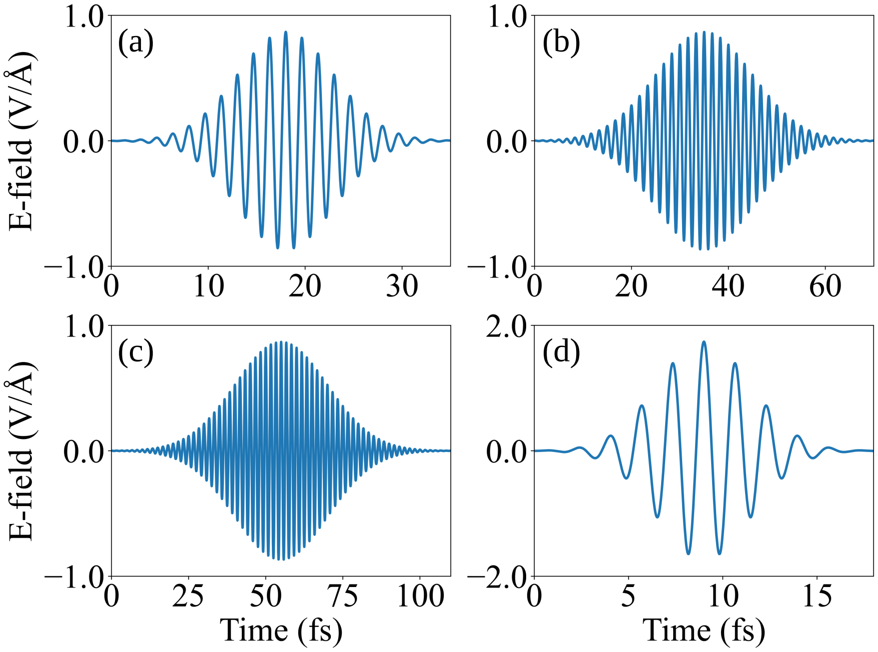

Figure S1: Electric field strength as a function of time for the four pulses used in this work (all four shown at plasmon frequency $\hbar\omega = \hbar\omega_p = 2.48$ eV): (a) pulse-1: $I_{\mathrm{max}} = 2 \times 10^{13}$ W cm^{-2} ($E_0 = 0.87$ V Å^{-1}), $t_0 = 18$ fs, $\sigma = 5$ fs, (b) pulse-2: $I_{\mathrm{max}} = 2 \times 10^{13}$ W cm^{-2}, $t_0 = 35$ fs, $\sigma = 10$ fs, (c) pulse-3: $I_{\mathrm{max}} = 2 \times 10^{13}$ W cm^{-2}, $t_0 = 55$ fs, $\sigma = 15$ fs, (d) pulse-4: $I_{\mathrm{max}} = 8 \times 10^{13}$ W cm^{-2} ($E_0 = 1.74$ V Å^{-1}), $t_0 = 9$ fs, $\sigma = 2.5$ fs.

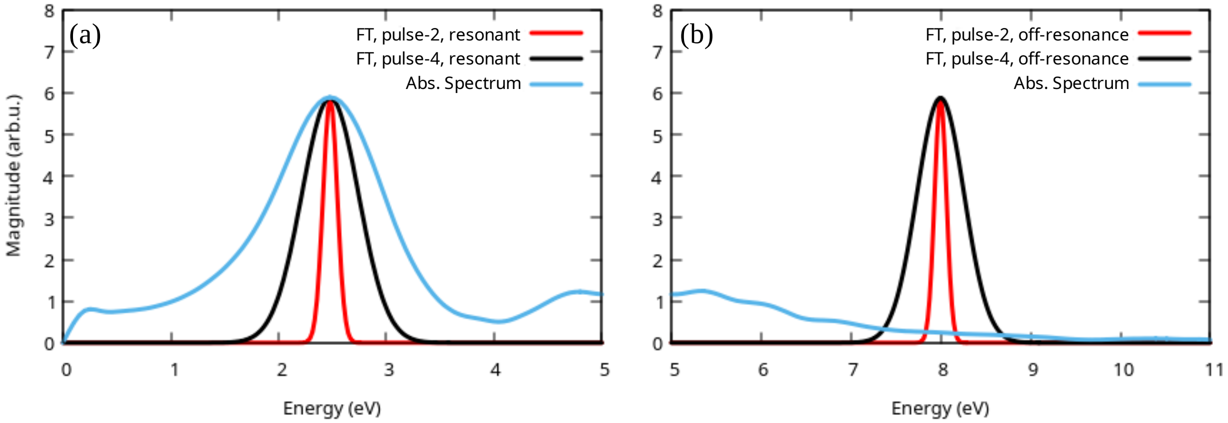

Figure S2: Spectral width obtained as a Fourier transform (FT) of the two pulses, pulse-2 ($\sigma = 10$ fs) and pulse-4 ($\sigma = 2.5$ fs) at (a) resonant frequency 2.48 eV, and (b) off-resonance frequency 8 eV, and compared to the absorption spectrum of the system. All the maxima are set to the same height.

S2 Induced dipole moment at low intensity

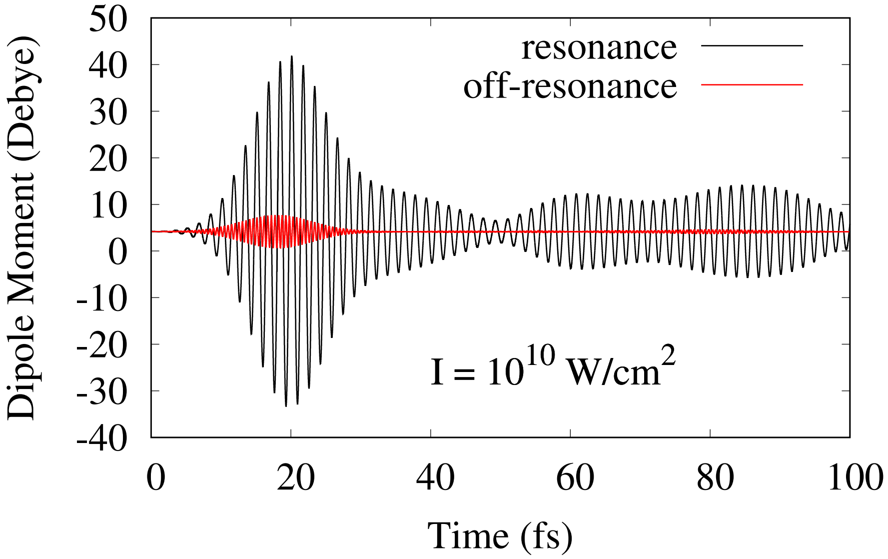

Figure S3: Time-dependent dipole moment induced in the Ag_{231}^{L1} nanoshell with H_2 adsorbate by the external pulse with intensity $I_{\max} = 2 \times 10^{10}$ W cm^{-2} and frequencies 2.48 eV (resonant condition) and 8 eV (off-resonance). The Gaussian pulse parameters are: $t_0 = 18$ fs, $\sigma = 5$ fs.

S3 Selected molecular orbitals

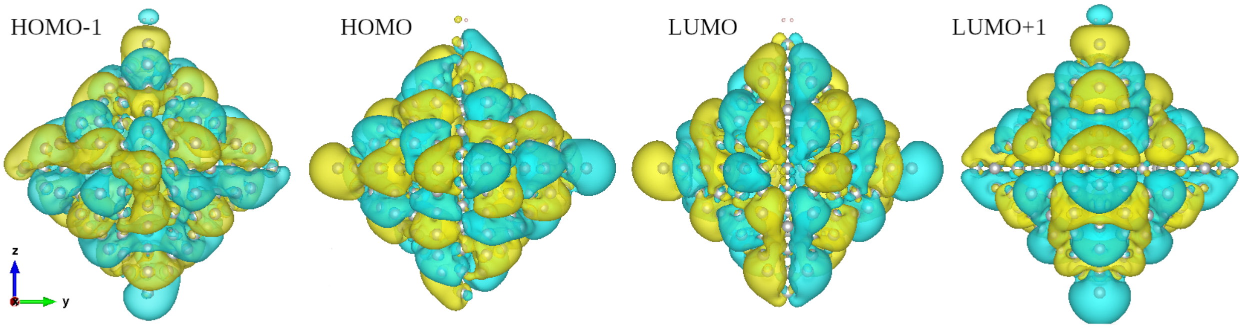

Figure S4: Ground-state molecular orbitals for the Ag_{231}^{L1} nanoshell with H_2 adsorbate.

S4 H_2 dissociation energy: gas-phase vs adsorbed

Figure S5 shows the potential energy as a function of the H-H internuclear distance for H_2 in gas-phase and H_2 adsorbed on the Ag_{231}^{L1} nanoshell. The energy is calculated using density functional theory (DFT) and the PBE exchange correlation functional with the CP2K software package. The calculated results are shown as symbols, while the extrapolated data is shown as lines. The potential energy at small (large) internuclear distances were calculated for a singlet (triplet) spin state of H_2 using unrestricted Kohn-Sham DFT with a spin multiplicity of 1 (3). For the triplet state of the adsorbed molecule, constrained DFT was employed to enforce the localization of spin-polarized electrons on the hydrogen atoms, ensuring a proper triplet configuration at large internuclear distances. The transition between the two spin states was captured by interpolating the energy using Akima spline extrapolation, providing a smooth transition between the singlet and triplet states.

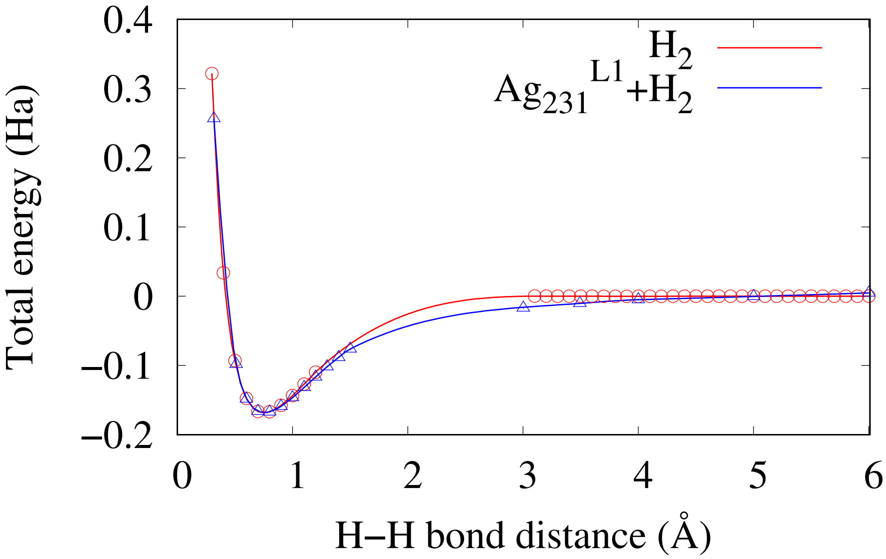

Figure S5: Potential energy (in Hartree units) as a function of the H-H internuclear distance for H_2 in gas-phase (red circles) and adsorbed on Ag_{231}^{L1} (blue triangles). Symbols show the DFT+PBE energies and lines represent the extrapolation of the calculated data.

S5 Population change on Ag_{231}^{L1} under pulses-1,-2,-3

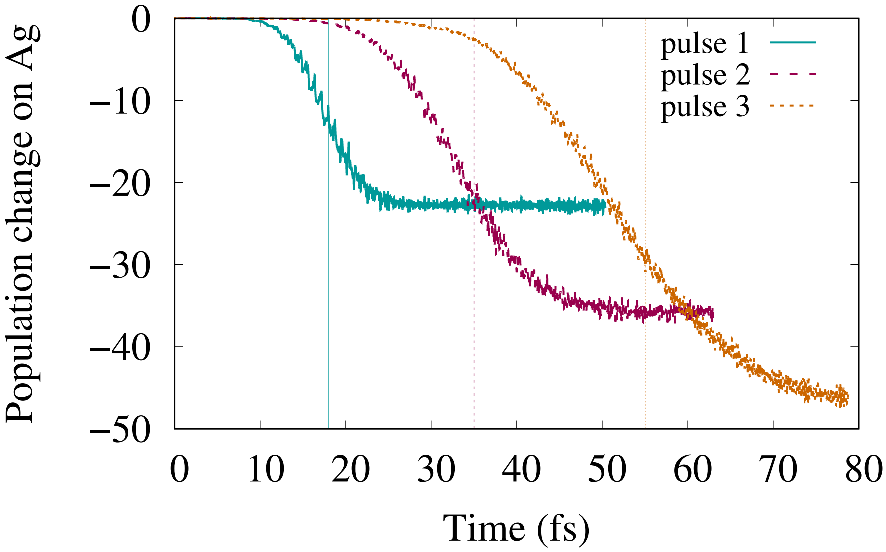

Figure S6: Mulliken population change $[\Delta N_e = N_e(t) - N_e(t = 0)]$ on Ag_{231}^{L1} nanoshell as a function of time for pulse-1, pulse-2, and pulse-3 (see pulses details in Fig. S1a-c) at frequency 2.48 eV.

S6 Dipole moment under pulse-4

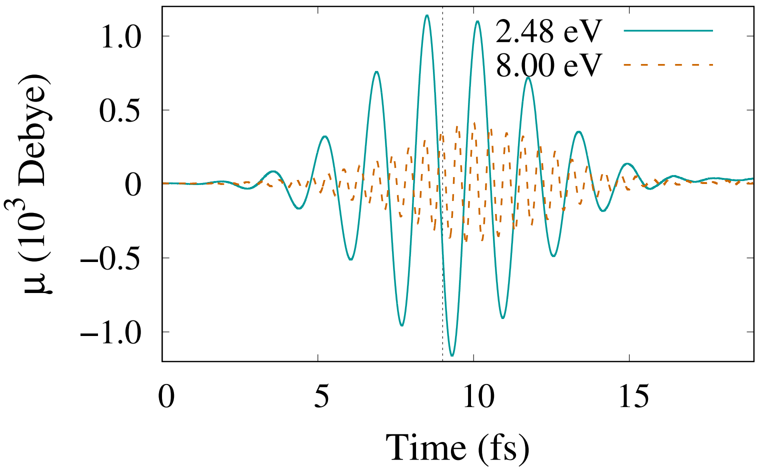

Figure S7: Time-dependent dipole moment for the Ag_{231}^{L1} nanoshell with H_2 adsorbate under the external pulse-4 with intensity $I_{max} = 8 \times 10^{13}$ W cm^{-2} and both frequencies. The vertical line shows the pulse maximum.

S7 H_2-Ag distance and population change on Ag_{231}^{L1} for pulses 2 and 4

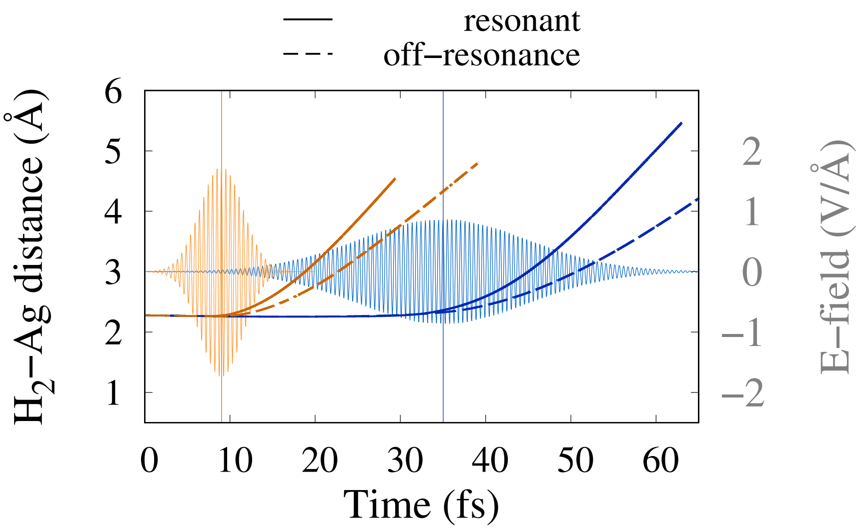

Figure S8: Time-dependent distance from the center of mass of H_2 to the top Ag atom of the Ag_{231}^{L1} nanoshell for pulse-2 (blue lines) and pulse-4 (orange lines) at frequencies $\hbar\omega = \hbar\omega_p = 2.48$ eV (solid lines) and $\hbar\omega = 8$ eV (dashed lines). Right-side Y-axis shows the field strength for the pulses. Note that H_2 dissociates in all the cases except for the off-resonant pulse-2 (see Fig. 5a of the main text).

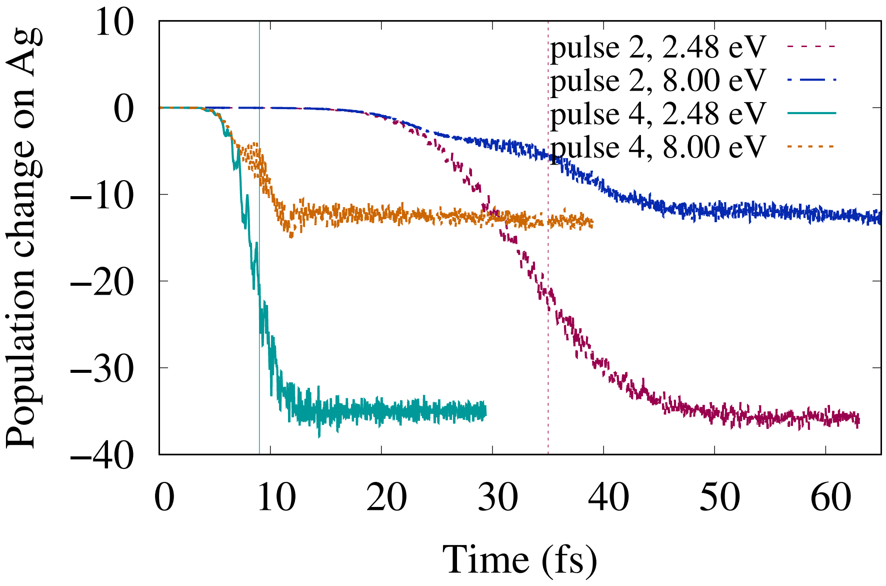

Figure S9: Mulliken population change $[\Delta N_e = N_e(t) - N_e(t=0)]$ on Ag_{231}^{L1} nanoshell as a function of time for pulse-4 compared to pulse-2 (see pulses details in Fig. S1b,d) at frequencies $\hbar\omega = \hbar\omega_\mathrm{p} = 2.48$ eV and $\hbar\omega = 8$ eV.

S8 Calculation of the induced electric field on Ag_{231}^{L1}+H_2

The induced charge density $\rho_\mathrm{ind}(\mathbf{r})$ generates an electrostatic potential $\Phi_\mathrm{ind}(\mathbf{r})$ governed by Poisson's equation:

$$\nabla^2\Phi_\mathrm{ind}(\mathbf{r}) = -4\pi\rho_\mathrm{ind}(\mathbf{r}), \tag{1}$$

where ϵ_0 is the vacuum permittivity. To solve this equation efficiently, we transform it into Fourier space. Taking the Fourier transform:

$$\mathcal{F}\left[\nabla^2\Phi_\mathrm{ind}(\mathbf{r})\right] = -4\pi\mathcal{F}\left[\rho_\mathrm{ind}(\mathbf{r})\right]. \tag{2}$$

Since the Fourier transform of the Laplacian is $-\mathbf{k}^2$, we obtain:

$$\tilde{\Phi}_\mathrm{ind}(\mathbf{k}) = \frac{4\pi\tilde{\rho}_\mathrm{ind}(\mathbf{k})}{k^2}, \tag{3}$$

where $\mathbf{k} = (k_x, k_y, k_z)$ is the wavevector, and $k^2 = k_x^2 + k_y^2 + k_z^2$.

The induced electric field is then given by:

$$\mathbf{E}_\mathrm{ind}(\mathbf{r}) = -\nabla\Phi_\mathrm{ind}(\mathbf{r}), \tag{4}$$

which, in Fourier space, becomes:

$$\tilde{\mathbf{E}}_\mathrm{ind}(\mathbf{k}) = -i\mathbf{k}\tilde{\Phi}_\mathrm{ind}(\mathbf{k}). \tag{5}$$

Substituting $\tilde{\Phi}_\mathrm{ind}(\mathbf{k})$:

$$\tilde{\mathbf{E}}_\mathrm{ind}(\mathbf{k}) = -i\mathbf{k}\frac{4\pi\tilde{\rho}_\mathrm{ind}(\mathbf{k})}{k^2}. \tag{6}$$

To avoid division by zero at $\mathbf{k} = 0$, we set $k^2 = 1$ at that point.

Finally, the induced field in real space is obtained via the inverse Fourier transform:

$$\mathbf{E}_{\text{ind}}(\mathbf{r}) = \mathcal{F}^{-1}\left[\tilde{\mathbf{E}}_{\text{ind}}(\mathbf{k})\right]. \tag{7}$$

Figure S10 shows the induced electric field on the Ag_{231}^{L1} nanoshell with H_2 adsorbate under the external pulse-1 with intensity $I_{\text{max}} = 2 \times 10^{13}$ W cm^{-2} and frequencies (left) 2.48 eV and (right) 8 eV at the time instant $t = 10$ fs. These results are obtained from the RT-TDDFT-ED calculations for the structures surrounded by the layer of ghost atoms. We show the mean over the $x-$axis induced field in the $yz-$plane. At the plasmon resonance (2.48 eV), the nanoparticle's collective oscillation strongly amplifies the external field, producing hot spots on the nanoshell vertices, with induced electric field in the vicinity of the H_2 molecule reaching 0.25 V Å^{-1}. In contrast, at the off-resonant excitation energy (8 eV), the particle's polarizability is much weaker and its induced field is largely out of phase with the driving field. As a result, there is a much weaker induced field at the H_2 location, reaching only about 0.05 V Å^{-1}, five time weaker than in the case of the resonant frequency.

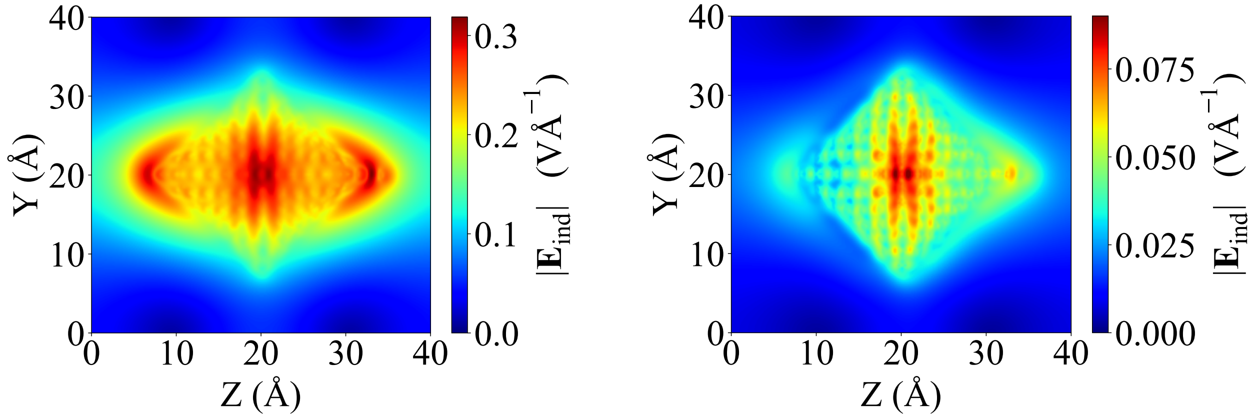

Figure S10: (z, y)-distribution of the x-averaged induced electric field $\langle \|\mathbf{E}_{\text{ind}}(y, z)\| \rangle_x$ on the Ag_{231}^{L1} nanoshell with H_2 adsorbed on the right vertex under the external pulse-1 with intensity $I_{\text{max}} = 2 \times 10^{13}$ W cm^{-2} and frequencies (left) 2.48 eV and (right) 8 eV at the time instant $t = 10$ fs. External field is polarized along the $z-$axis. Notice different scale.

The electron oscillations due to plasmon translate into a symmetrical induced field distribution around both vertices along the $z-$axis in Fig. S10(left) due to the fact that we show the modulus $\langle \|\mathbf{E}_{\text{ind}}\| \rangle_x$. Since strong field of the pulses leads to the superposition of both plasmonic and nonlinear effects such as ionization, the observed symmetry is lost at the time instances when the nanoshell has lost electrons (Figs. S13, S14, S17, S18, and S21 below). The emitted electrons occupy ghost atoms in the time-dependent density, while all the electrons are on the Ag_{231}^{L1}+ H_2 in the ground-state density (for the current snapshot atomic structure) which we subtract to find the induced density. This means that the positive electron change on one vertex will be smaller than the negative electron change on the other vertex by the number of emitted electrons.

S9 External electric field and induced dipole moment for pulses 2 and 4

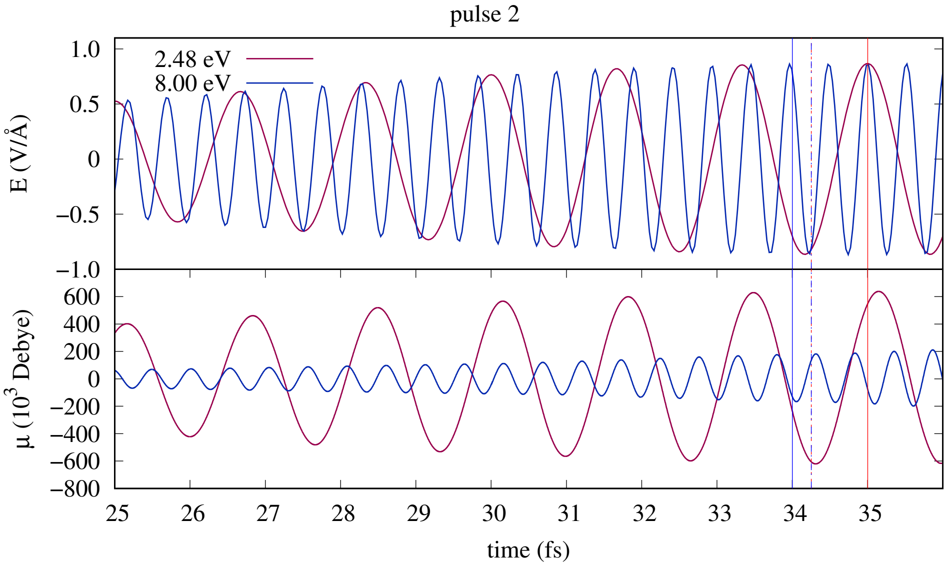

Figure S11: Upper panel: Electric field strength for pulse-2 with frequencies 2.48 eV (resonant) and 8 eV (off-resonant). Lower panel: Corresponding induced dipole moment as a function of time. Vertical red (blue) lines show the time instances used for plotting the induced electric field at 2.48 eV (8 eV) in Fig. 6 of the main article and in Figs S13 to S16 below.

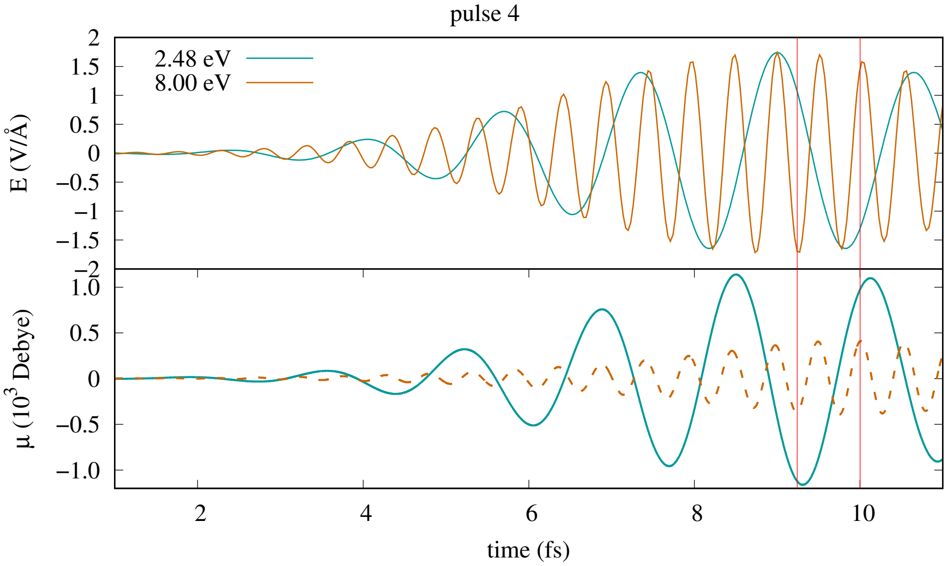

Figure S12: Same as Fig. S11 for pulse-4 corresponding to Fig. 7 of the main article and to Figs S17 to S20 below.

S10 Induced electric field analysis at the position of H_2

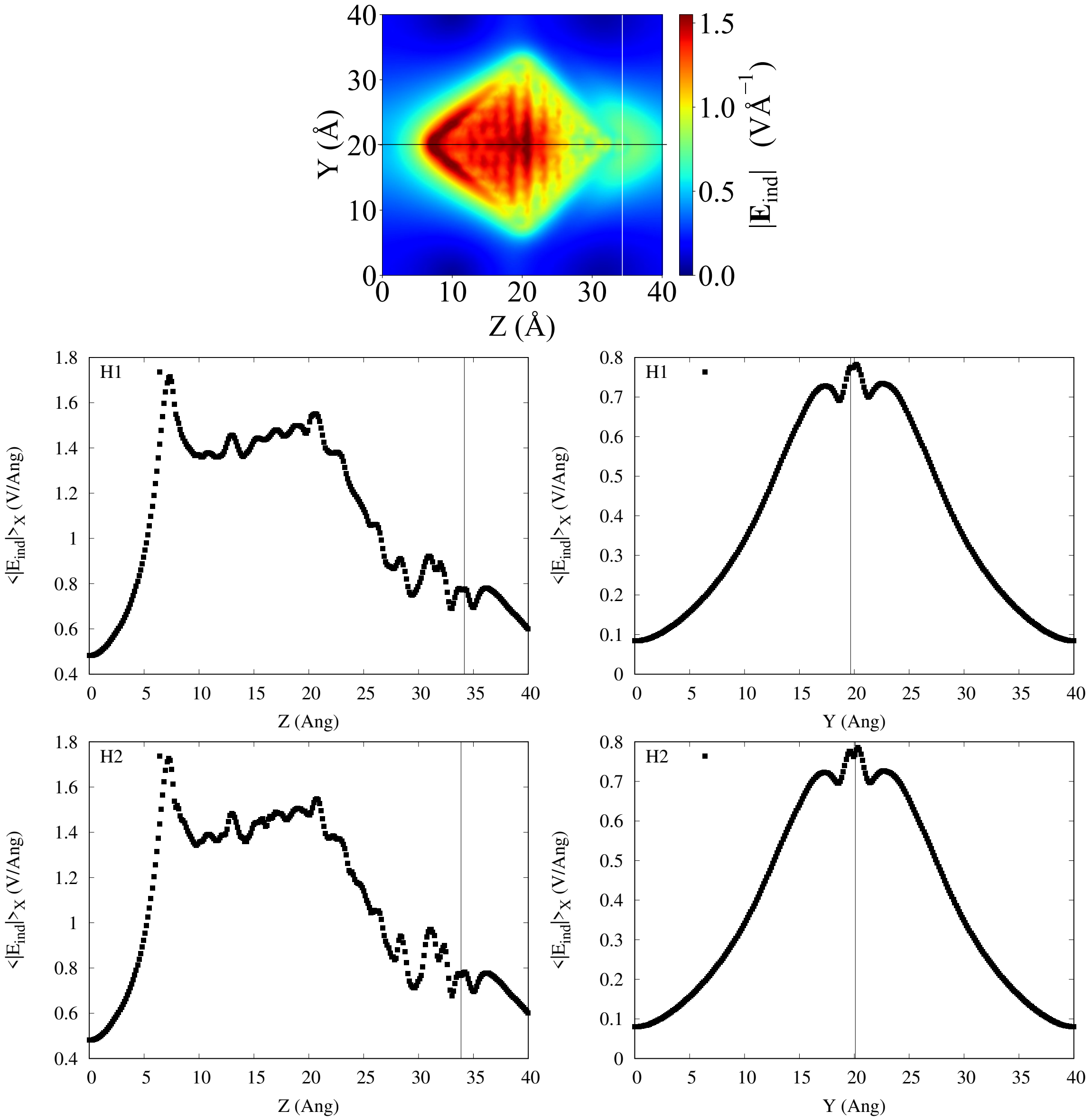

Figure S13: x-averaged electric field induced on Ag_{231}^{L1}+H_2 by the external pulse-2 with frequency 2.48 eV at the time instant $t = 34.25$ fs. The molecule is adsorbed on the right vertex. The Cartesian coordinates of the atoms forming the molecule, denoted as H1 and H2 in the figure, are (20.17091, 19.65791, 34.16472) and (19.41151, 20.09346, 33.86330), respectively. (Upper panel) (z, y)-distribution of the x-averaged induced electric field. Horizontal (vertical) black (white) line approximately shows the cut through H1 and H2 at their y (z) positions, for which lower left (lower right) panels show the induced electric field as a function of z (y).

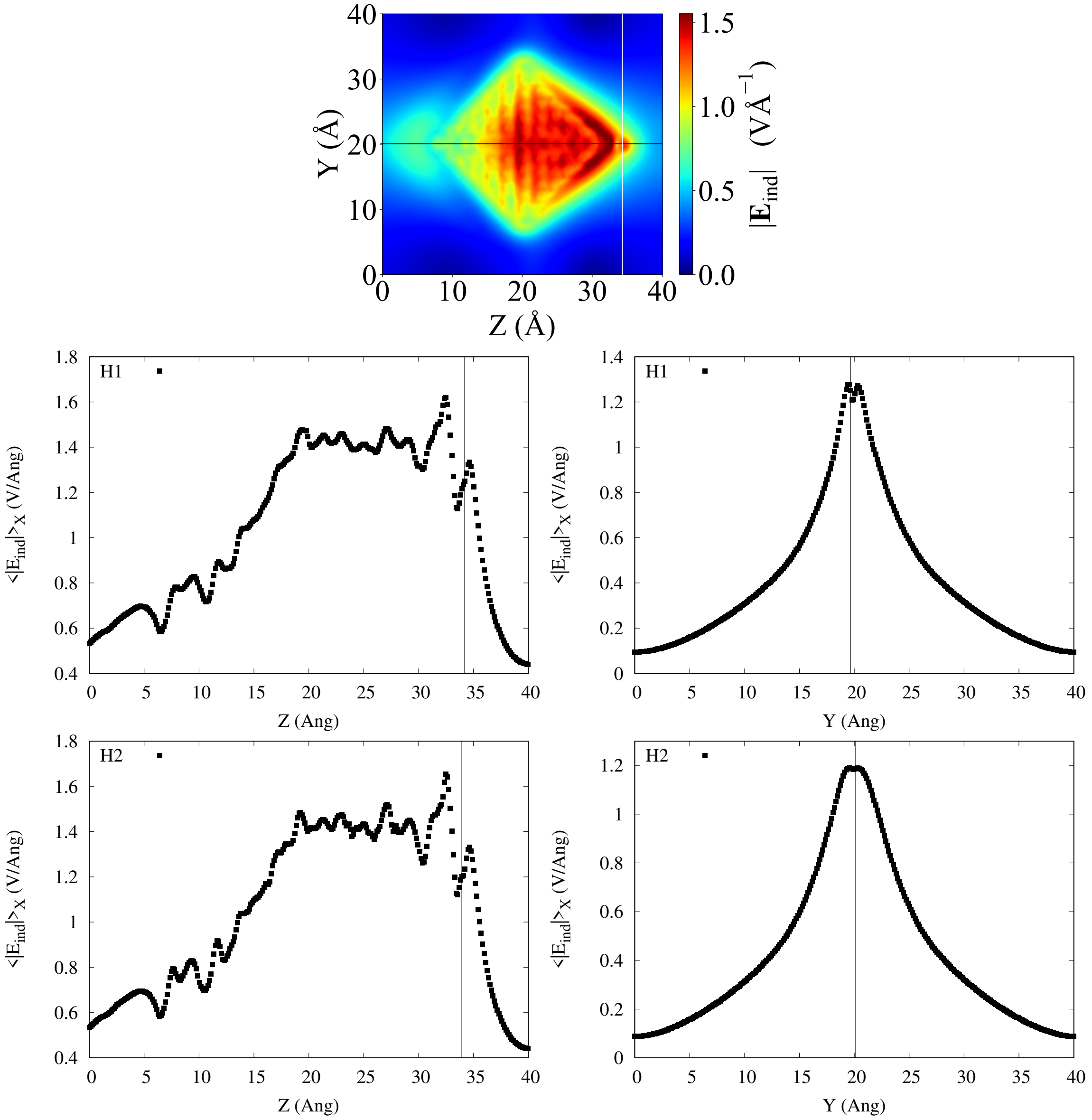

Figure S14: Same as Fig. S13 but for pulse-2 with frequency 2.48 eV at the time instant $t = 35$ fs. The molecule Cartesian coordinates are H1: (20.16494 19.66330 34.18505) and H2: (19.39228, 20.08282, 33.88200).

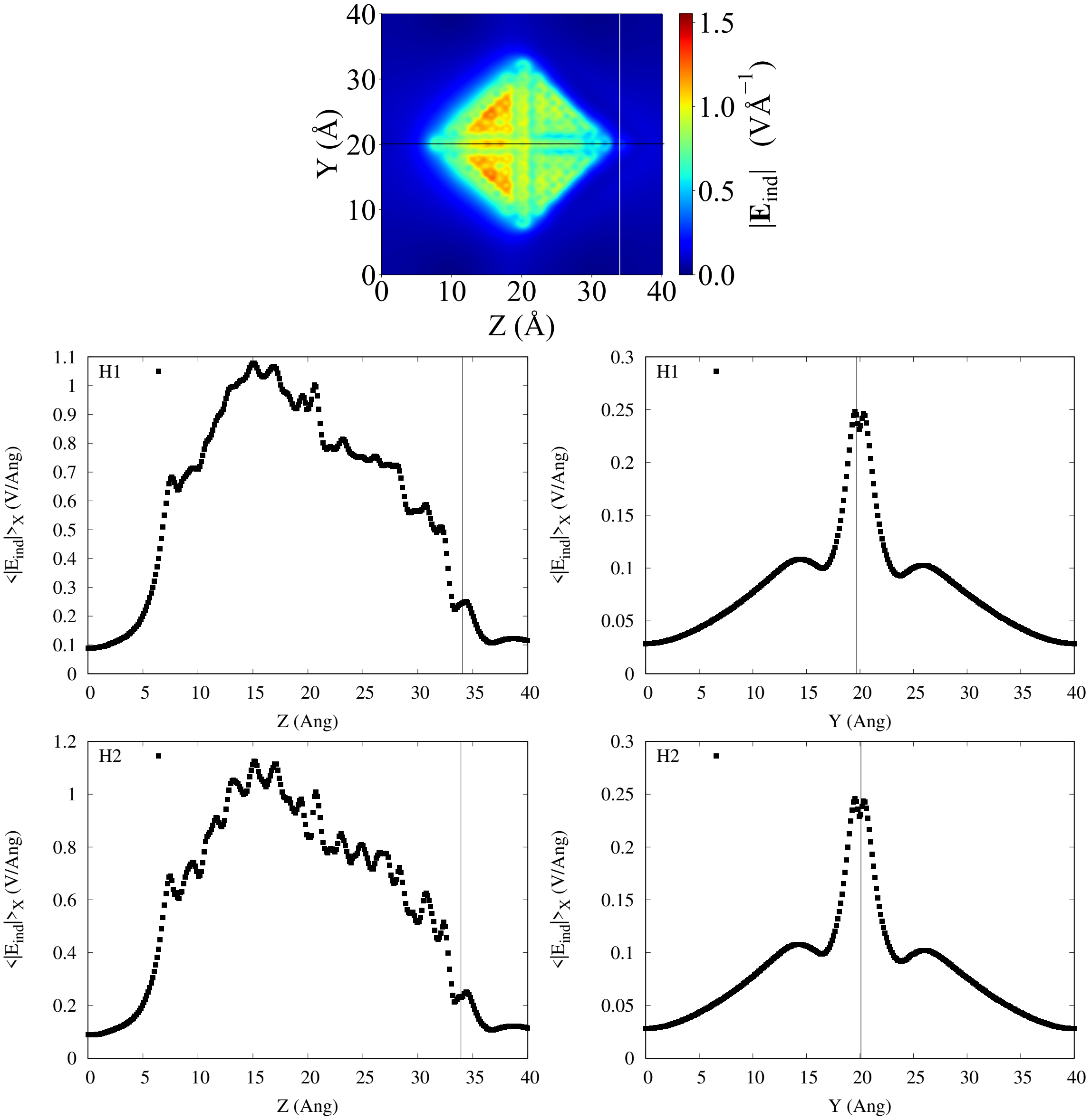

Figure S15: Same as Fig. S13 but for pulse-2 with frequency 8 eV at the time instant $t = 34$ fs. The molecule Cartesian coordinates are H1: (20.13996, 19.67609, 34.05631) and H2: (19.45773, 20.08741, 33.91462).

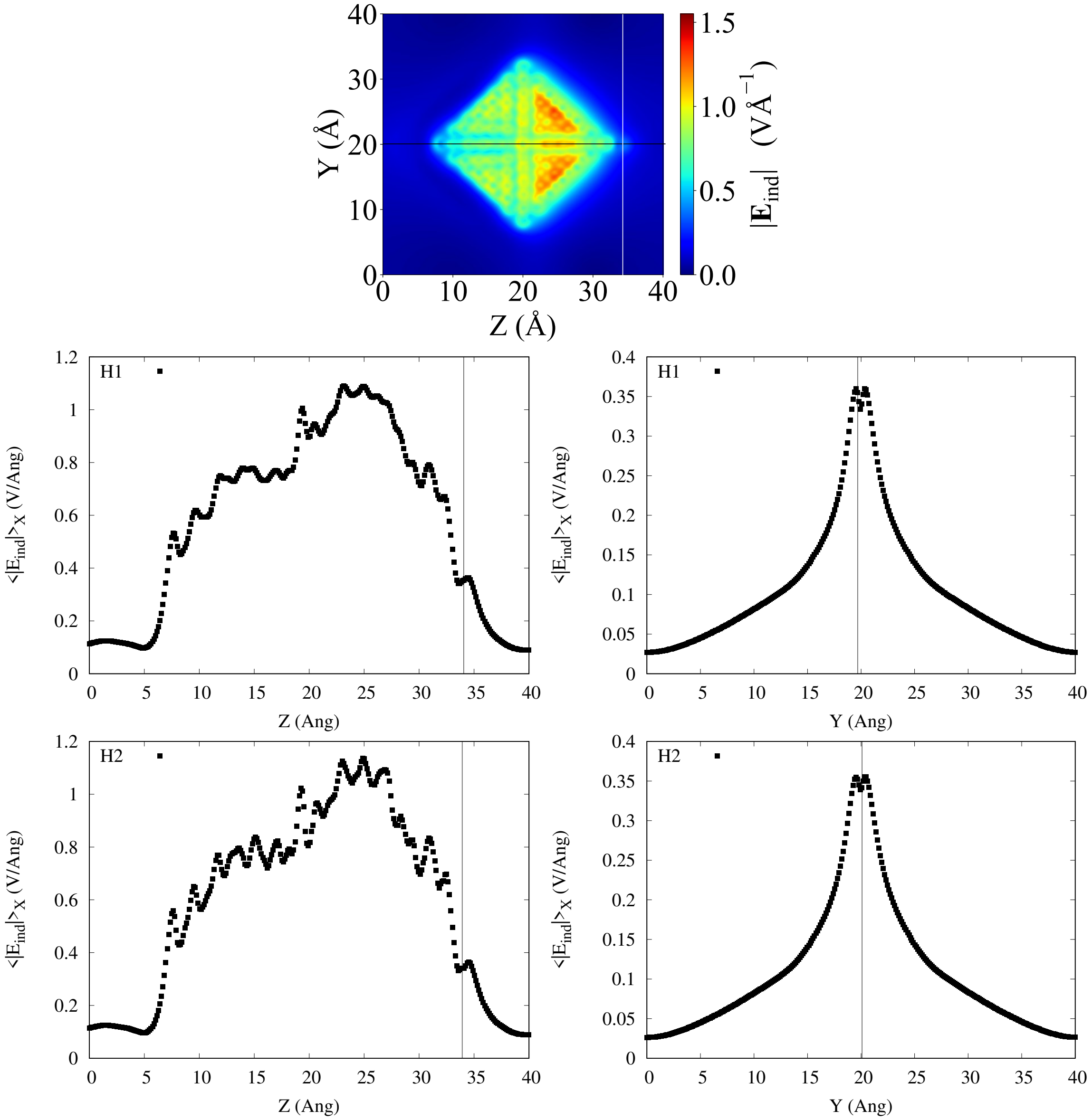

Figure S16: Same as Fig. S13 but for pulse-2 with frequency 8 eV at the time instant $t = 34.25$ fs. The molecule Cartesian coordinates are H1: (20.13695, 19.67874, 34.05676) and H2: (19.45385, 20.08326, 33.91865).

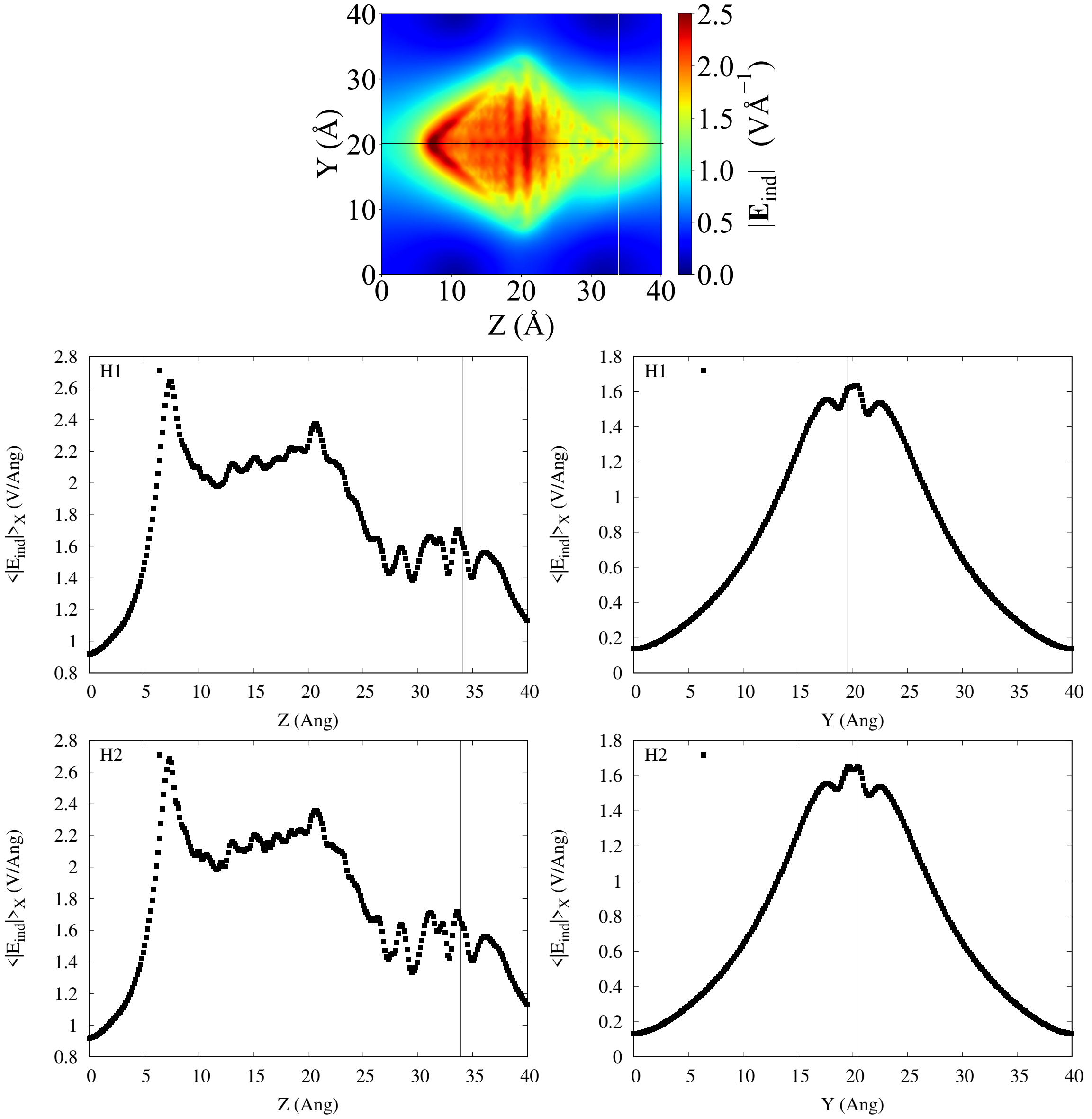

Figure S17: Same as Fig. S13 but for pulse-4 with frequency 2.48 eV at the time instant $t = 9.24$ fs. The molecule Cartesian coordinates are H1: (20.17667, 19.53189, 34.10876) and H2: (20.04871, 20.39224, 33.92203).

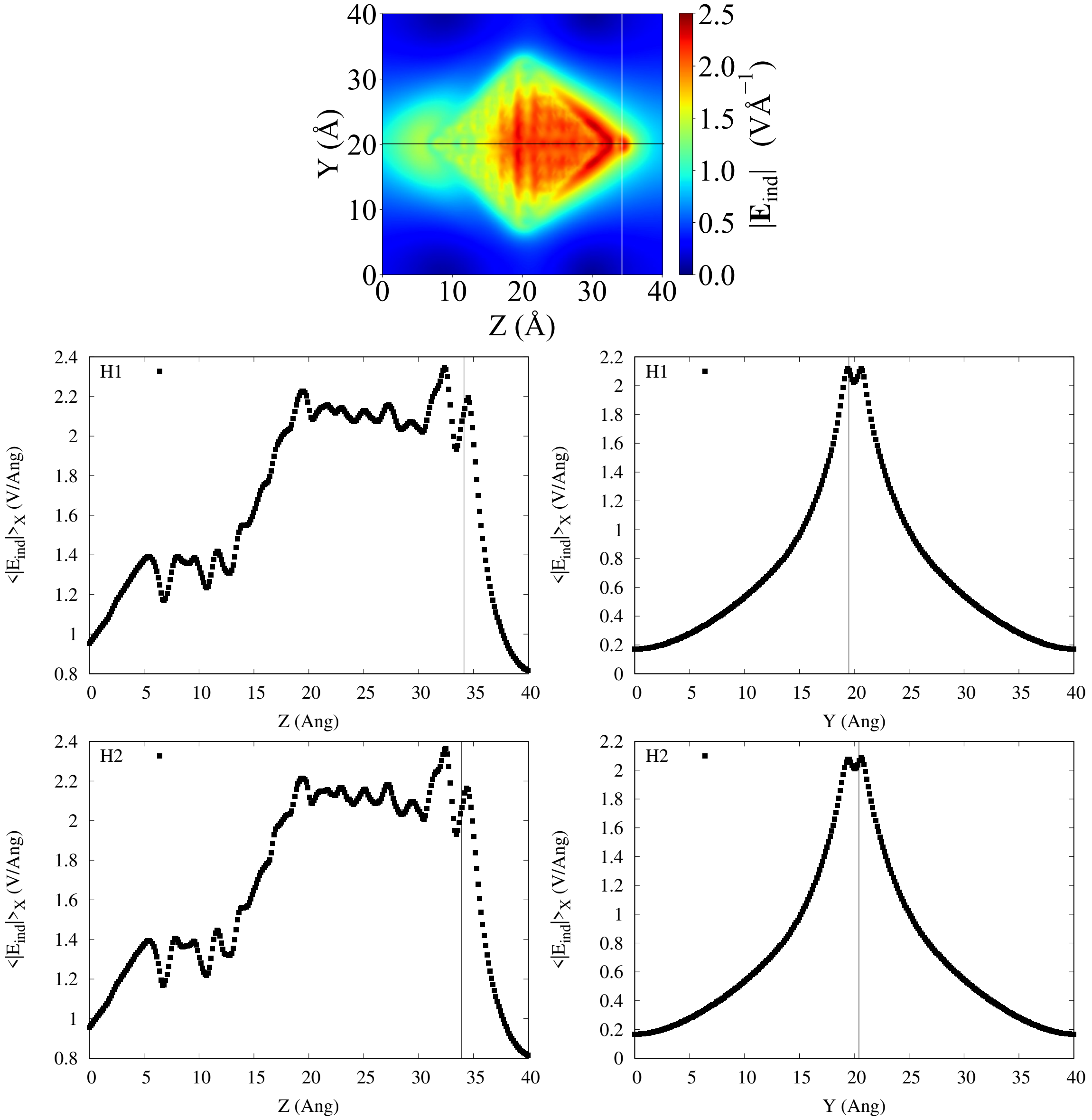

Figure S18: Same as Fig. S13 but for pulse-4 with frequency 2.48 eV at the time instant $t = 10$ fs. The molecule Cartesian coordinates are H1: (20.18015, 19.49985, 34.13747) and H2: (20.02655, 20.42064, 33.92358).

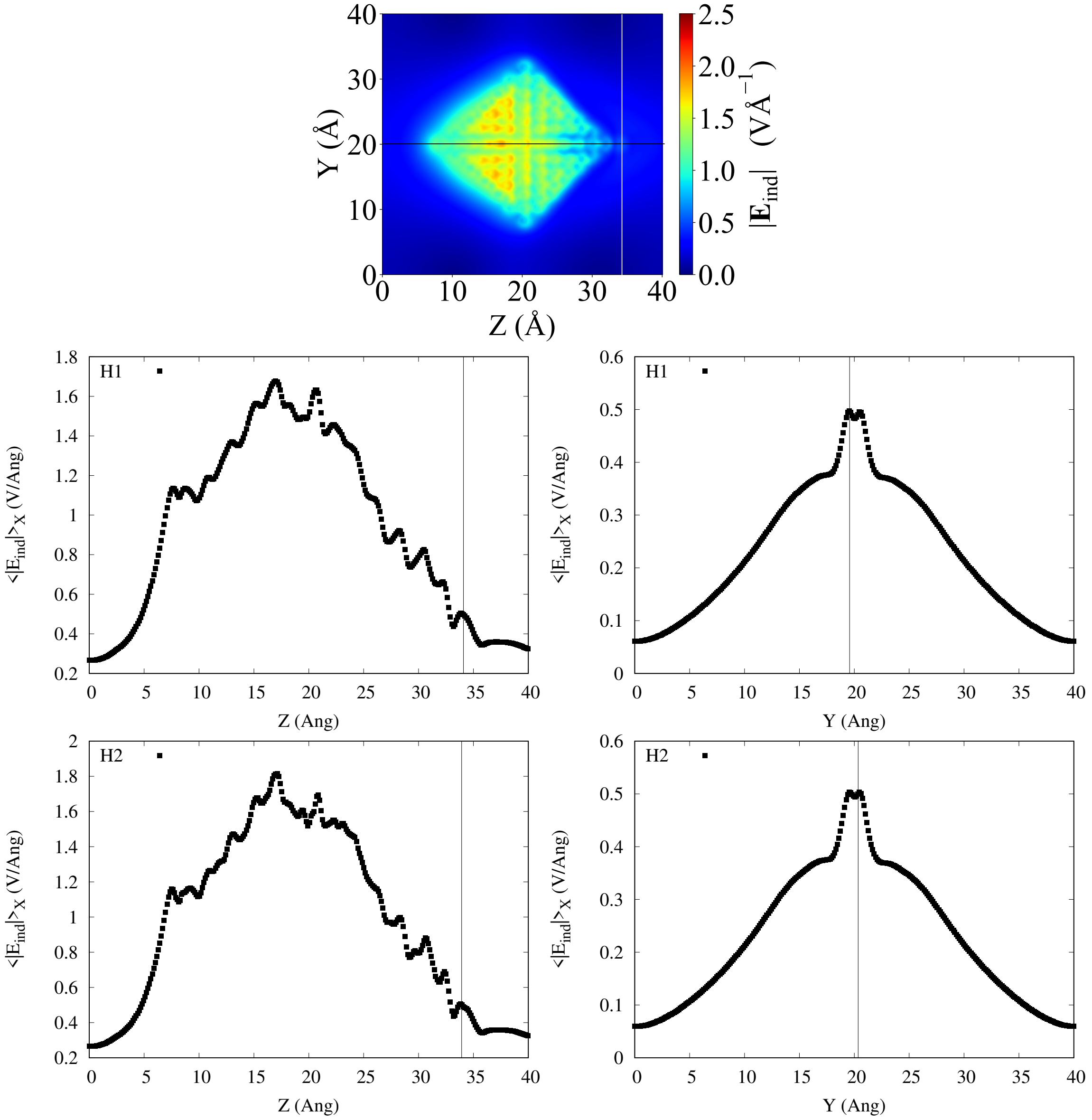

Figure S19: Same as Fig. S13 but for pulse-4 with frequency 8 eV at the time instant $t = 9.24$ fs. The molecule Cartesian coordinates are H1: (20.17310, 19.56901, 34.08232) and H2: (20.05217, 20.35282, 33.92159).

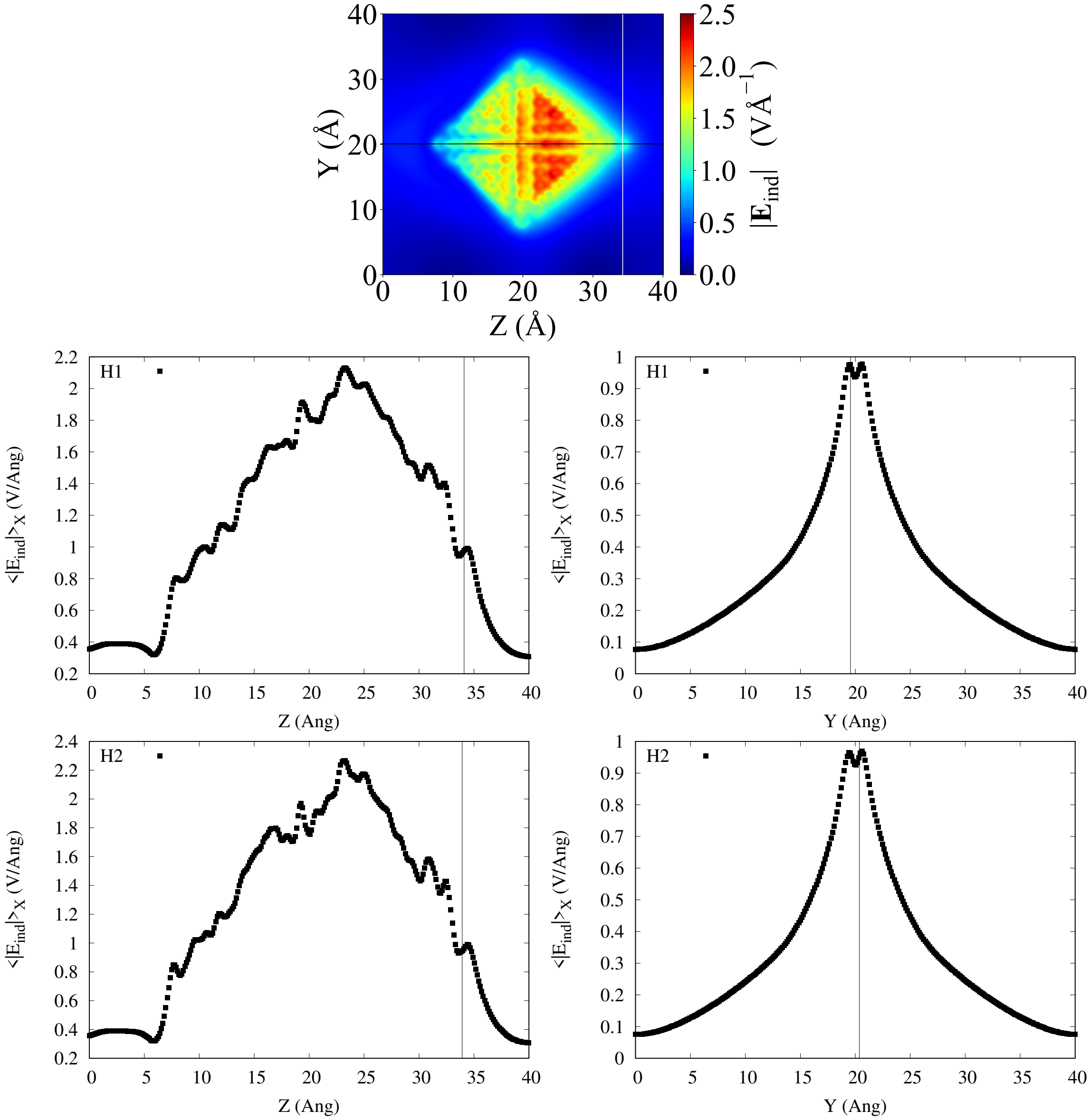

Figure S20: Same as Fig. S13 but for pulse-4 with frequency 8 eV at the time instant $t = 10$ fs. The molecule Cartesian coordinates are H1: (20.17441, 19.55348, 34.09393) and H2: (20.03204, 20.36180, 33.91831).

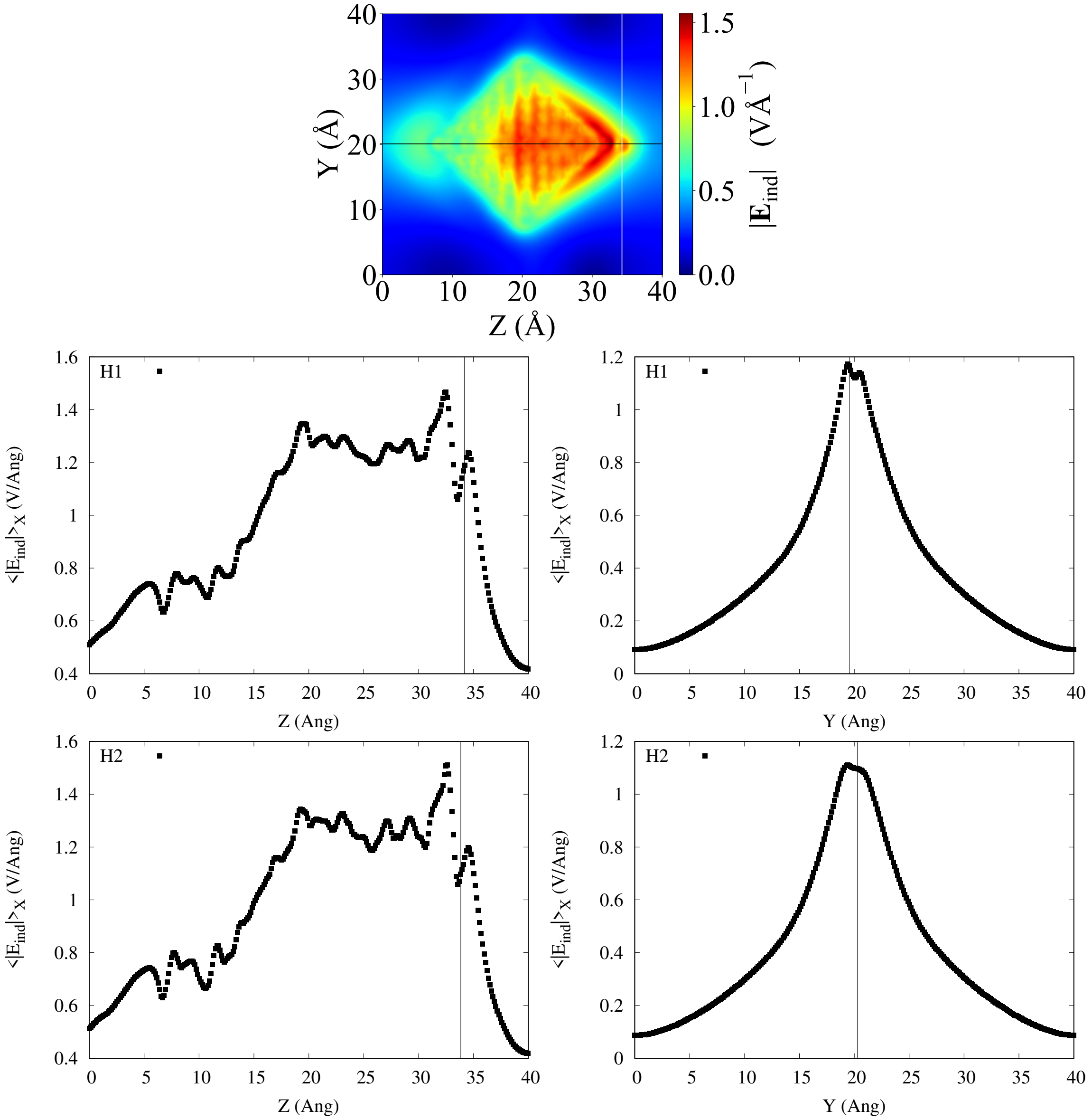

Figure S21: Same as Fig. S13 but for pulse-1 with frequency 2.48 eV at the time instant $t = 20$ fs. The molecule Cartesian coordinates are H1: (20.17377, 19.56827, 34.15810) and H2: (19.77894, 20.27348, 33.84442).

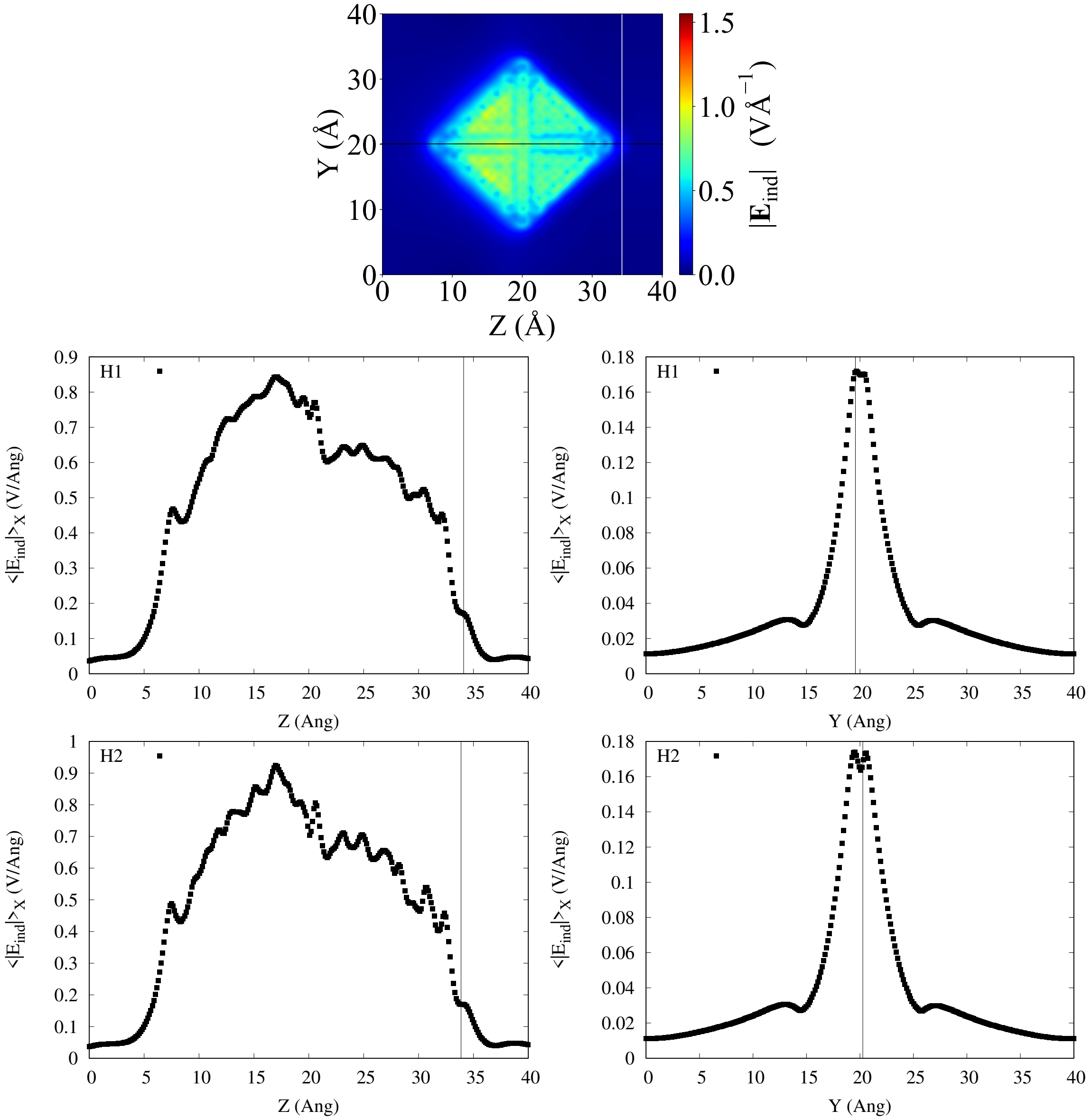

Figure S22: Same as Fig. S13 but for pulse-1 with frequency 8 eV at the time instant $t = 20$ fs. The molecule Cartesian coordinates are H1: (20.17020, 19.57946, 34.10292) and H2: (19.78535, 20.26223, 33.86742).

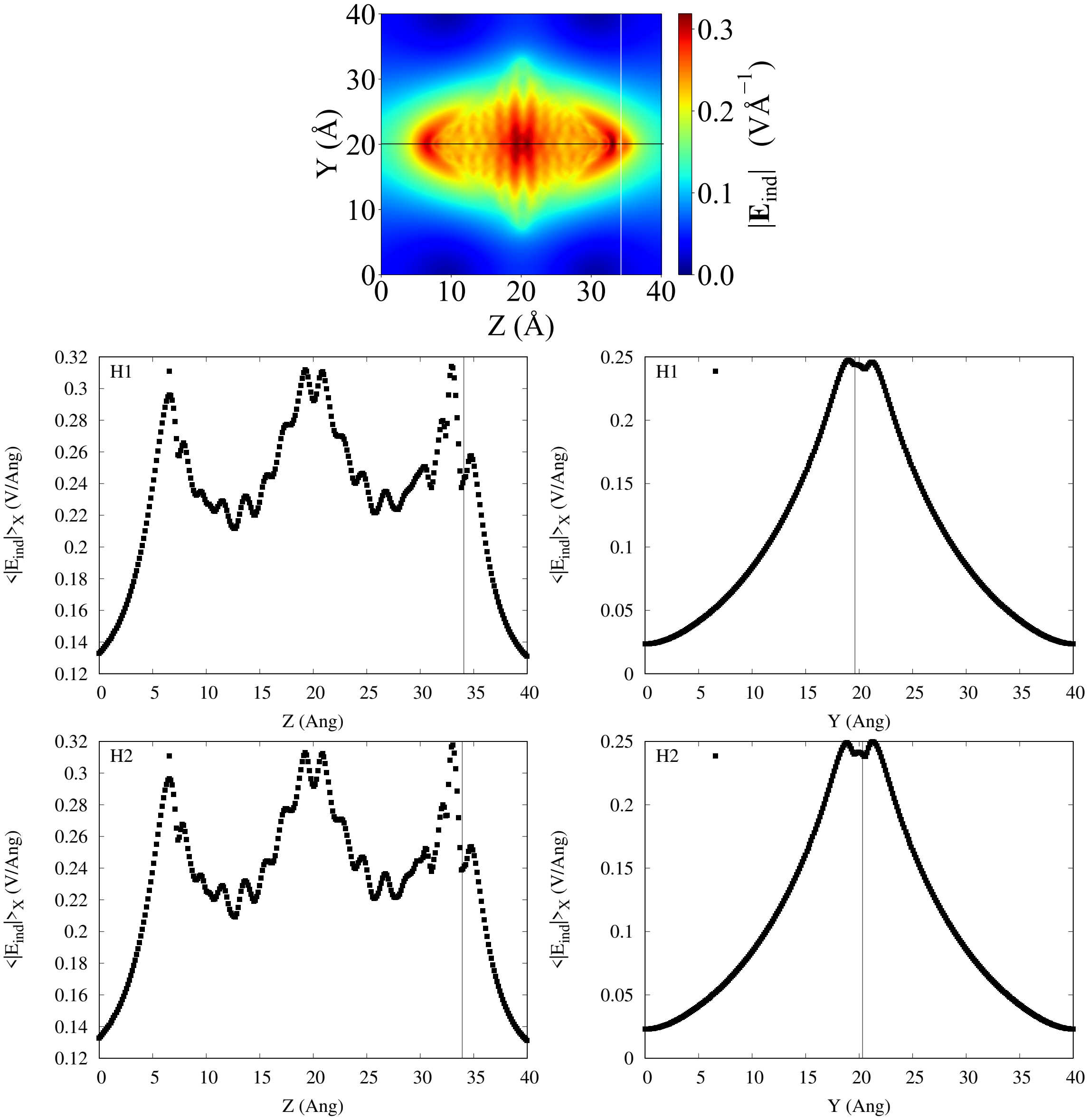

Figure S23: Same as Fig. S13 but for pulse-1 with frequency 2.48 eV at the time instant $t = 10$ fs. The molecule Cartesian coordinates are H1: (20.17012, 19.60066, 34.07398) and H2: (20.03598, 20.31432, 33.91182).

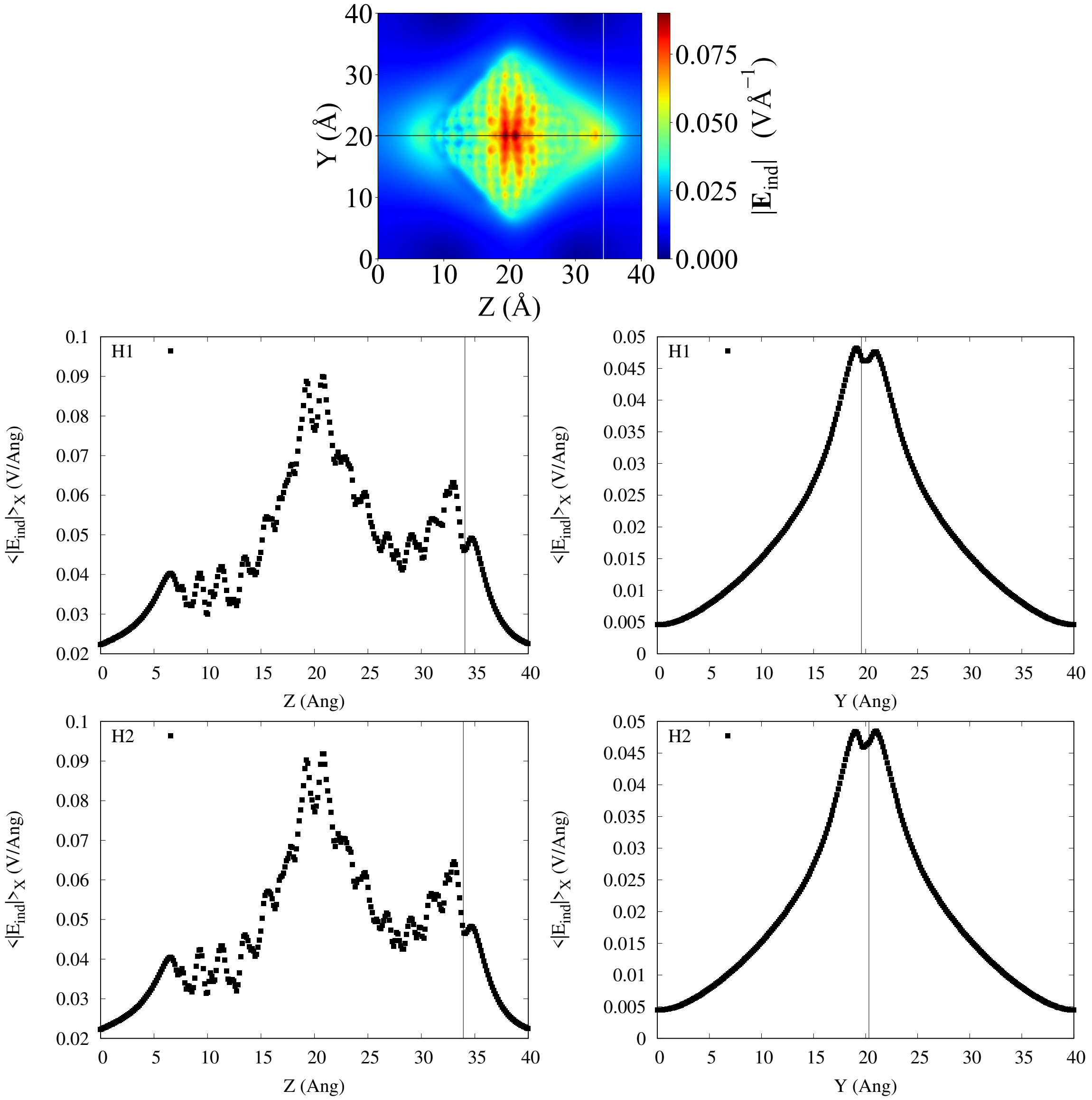

Figure S24: Same as Fig. S13 but for pulse-1 with frequency 8 eV at the time instant $t = 10$ fs. The molecule Cartesian coordinates are H1: (20.17003, 19.60123, 34.07358) and H2: (20.03605, 20.31386, 33.91217).

S11 Cartesian coordinates of the Ag_{231}^{L1}+H_2 with the ghost atomic layer

Below, the cartesian coordinates of the system studied in this work are presented in the Å units (XYZ format). The first column indicates the atomic species labels, where Ag_g labels represent ghost atoms. The labels column is followed but the x, y, and z coordinates.

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Ag	10.3969324580	18.4704803605	19.9749733459
Ag	9.8801398143	20.0022852738	17.6904280306
Ag	8.0888818953	20.0024411773	19.9661760238
Ag	9.8556055227	20.0016089713	22.2540382774
Ag	10.3978188286	21.5330803014	19.9753907810
Ag	14.2886254244	14.4888567043	19.9924349493
Ag	11.7402234422	17.8383556081	17.6089306887
Ag	13.6352454232	15.7706074735	17.5819324604
Ag	13.5269919275	17.6297445297	15.4621406523
Ag	12.3458745851	16.4772986766	19.9842201854
Ag	11.6989611913	17.8219232675	22.3604611125
Ag	13.6078006115	15.7654472226	22.3992529023
Ag	13.4785233200	17.6281848211	24.5147023512
Ag	14.1436803508	20.0013865510	14.0739738942
Ag	12.0640398151	20.0016094902	15.8964524609
Ag	11.7414159352	22.1648828099	17.6092539738
Ag	13.5272995214	22.3731781996	15.4617026651
Ag	11.6981893513	22.1818846868	22.3618166025
Ag	12.0312307647	20.0014735977	24.0499984880
Ag	14.0643951367	20.0010738844	25.9209190860
Ag	13.4771370672	22.3750962462	24.5169470349
Ag	13.6388776091	24.2301550132	17.5831828044
Ag	12.3487427238	23.5240662974	19.9851331769
Ag	13.6086928479	24.2367423285	22.4008273148
Ag	14.2924551674	25.5114332611	19.9937634217
Ag	17.8613920942	10.1968600653	20.0091246164
Ag	15.5833951804	13.7595916313	17.6063098304
Ag	17.6327325695	11.8275271298	17.7153300309
Ag	17.5973572817	13.7201300116	15.6501444517
Ag	16.1054697776	12.3628514861	19.9997203404
Ag	15.5659524087	13.7638967259	22.3871670326
Ag	17.6222898370	11.8433394721	22.2940101453
Ag	17.5785553640	13.7515552124	24.3421728593
Ag	15.5685586228	17.6231500519	13.5397269162
Ag	17.5992348097	15.6819554995	13.6520342625
Ag	17.6623079684	17.6744907698	11.6681230928
Ag	15.4452894919	15.5452454280	15.4367815433

Ag	15.4081735825	15.5542970523	24.5532216470
Ag	15.5002627634	17.6264323741	26.4579311622
Ag	17.5728934575	15.7309048904	26.3211906509
Ag	17.5959168744	17.6972556276	28.3280868666
Ag	17.9687630717	20.0003788215	10.0782356772
Ag	16.1364672231	20.0012298990	12.1546042066
Ag	15.5681732197	22.3799444461	13.5385146442
Ag	17.6619432191	22.3276815121	11.6668410117
Ag	15.4994562590	22.3757058343	26.4598213858
Ag	16.0389483499	20.0005404778	27.8575723089
Ag	17.7972375005	19.9997184114	30.0050481369
Ag	17.5956879009	22.3034157438	28.3293938547
Ag	17.5989592720	24.3213350809	13.6497422430
Ag	15.4461983646	24.4572988722	15.4361266637
Ag	15.5870395016	26.2407002191	17.6074090800
Ag	17.5976881884	26.2831832316	15.6479342060
Ag	15.5671683337	26.2378924126	22.3892450548
Ag	15.4076820718	24.4483737609	24.5559174465
Ag	17.5726229605	24.2708769460	26.3236414934
Ag	17.5786017421	26.2506890541	24.3451500946
Ag	17.6342476449	28.1745087219	17.7145912110
Ag	16.1101716773	27.6364694049	20.0009574387
Ag	17.6230662931	28.1591105712	22.2970147056
Ag	17.8661729710	29.8017229587	20.0098888082
Ag	19.9665275763	10.2943560157	18.1476541743
Ag	19.9312977659	8.2487443974	20.0217294263
Ag	19.9615075155	10.3156131430	21.8713429548
Ag	22.0610040189	10.0732678730	20.0132194210
Ag	20.0059587165	14.3912915084	14.4007439375
Ag	19.9859367859	12.3699752741	16.3030506070
Ag	22.3545586352	11.6660913609	17.6843087284
Ag	22.4110273407	13.6511226423	15.6919077545
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Ag_g	9.7751607843	19.9999999999	26.1347523823
Ag_g	9.7751607835	20.0000000006	13.8652476171
Ag_g	30.2248392174	19.9999999995	13.8652476159
Ag_g	32.2697596974	19.9999999998	24.0898752286
Ag_g	7.7302403039	19.9999999992	15.9101247741
Ag_g	7.7302403014	20.0000000008	24.0898752297
Ag_g	32.2697596975	19.9999999997	15.9101247742
Ag_g	34.3147335795	20.0000000000	22.0447127785
Ag_g	5.6852664202	20.0000000003	22.0447127783
Ag_g	5.6852664190	19.9999999996	17.9552872207
Ag_g	34.3147335809	19.9999999999	17.9552872212
Ag_g	36.3599272377	20.0000000001	19.9999999995
Ag_g	3.6400727625	20.0000000002	20.0000000000

Ag_g	26.1348574258	11.8202139258	22.0448201273
Ag_g	26.1348574226	11.8202139274	17.9551798722
Ag_g	26.1348574263	28.1797860727	22.0448201280
Ag_g	26.1348574217	28.1797860719	17.9551798664
Ag_g	13.8651425742	28.1797860754	22.0448201245
Ag_g	13.8651425764	28.1797860705	17.9551798734
Ag_g	13.8651425805	11.8202139311	22.0448201314
Ag_g	13.8651425758	11.8202139260	17.9551798718
Ag_g	20.0000000000	20.0000000003	3.6400727625