Supplementary Information

Interstellar Ice Embedded Glycine Response to H^+/proton Irradiation. A Theoretical Study

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A Benchmark Study

All three DFT parameters, that are the basis set, auxiliary basis and XC functional were chosen from a complete benchmark study conducted specifically for this research from a compromise between accuracy and computational cost. The benchmark calculations on the comparison between deposited energies and charge migration evolution was carried out for H^+ 1keV collision on isolated N-Gly molecular system. In a first place, PBE96 XC-functional was fixed, and six different basis set were employed (STO3G, DZVP, 611++G(2p2d),aug-*cc*-PVDZ, def2-TZVP and TZVP). It must be precised that for each basis set used, two different auxiliary basis set were considered (GEN-A2 and GEN-A2*).

Figure S1 plots the deposit energy distributions. It can be observed that, apart from DZVP and STO3G, deposit energy distribution do not vary noteably. Similarly, Figure S2 presents the charge migration distribution for different parameters. In this case, all the basis sets yielded highly comparable charge distribution profiles. Finaly, from the computational cost analysis (see Figure S3) it was conclude that TZVP basis set are a good compromise between accuracy of the electronic dynamics simulations and computations expenses.

An additional benchamrk was carried out on a set of H^+ 1keV collision simulations on N-Gly-4H_2O molecular system. The comparisons of the deposited energies for the six types of bases (see Figure S4) confirmed the conclusion that TZVP basis set with GEN-A2 auxiliary basis and PBE96 XC-functional is the more convenient set of parameters to be used in our research.

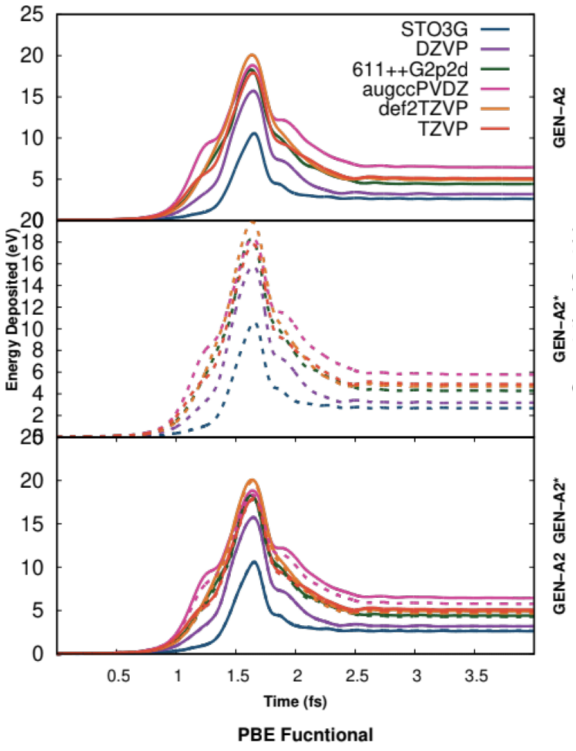

Fig. S1 Comparison of energy deposition curve for basis set benchmark. Collision simulations modeling N-Gly isolated molecule using PBE96 XC-functional, GEN-A2 and GEN-A2* and six different basis set: STO3G (blue), DZVP (purple), 611++G(2p2d) (green), aug-*cc*-PVDZ (pink), def2-TZVP (orange) and TZVP (red).

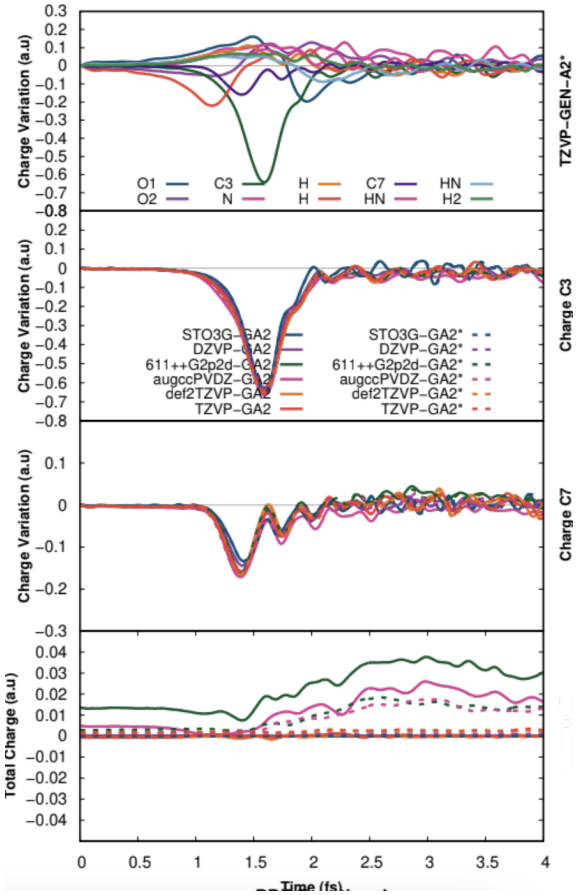

Fig. S2 Charge variation benchmark comparison. Collision simulations modeling N-Gly isolated molecule using PBE96 XC-functional, GEN-A2 and GEN-A2* and six different basis set: STO3G (blue), DZVP (purple), 611++G(2p2d) (green), aug-*cc*-PVDZ (pink), def2-TZVP (orange) and TZVP (red).

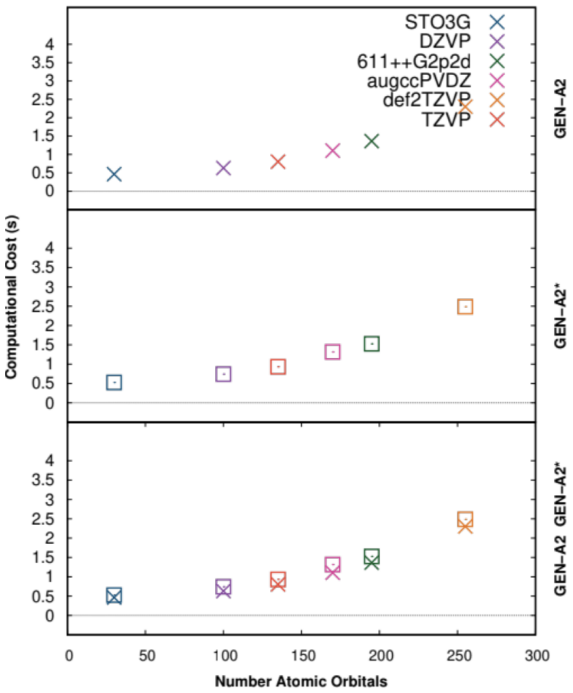

Fig. S3 Computational cost benchmark. Collision simulations modeling N-Gly isolated molecule using PBE96 XC-functional, GEN-A2 and GEN-A2* and six different basis set: STO3G (blue), DZVP (purple), 611++G(2p2d) (green), aug-*cc*-PVDZ (pink), def2-TZVP (orange) and TZVP (red).

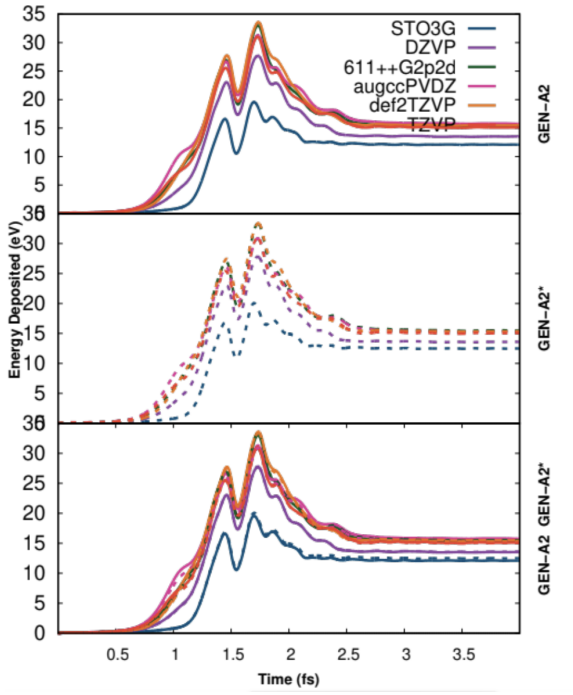

Fig. S4 Comparison of energy deposition curve for basis set benchmark. Collision simulations modeling Gly-4H_2O molecular cluster using PBE96 XC-functional, GEN-A2 and GEN-A2* and six different basis set: STO3G (blue), DZVP (purple), 611++G(2p2d) (green), aug-*cc*-PVDZ (pink), def2-TZVP (orange) and TZVP (red).

B Electron dynamic simulation time step benchmark

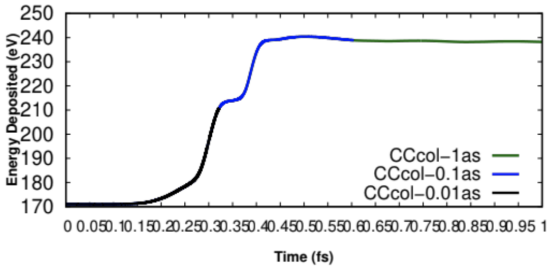

Fig. S5 Electronic time step simulation time study for N-Gly-LDA H^+ 100keV collision process.

C Supplementary models and projectile orientations

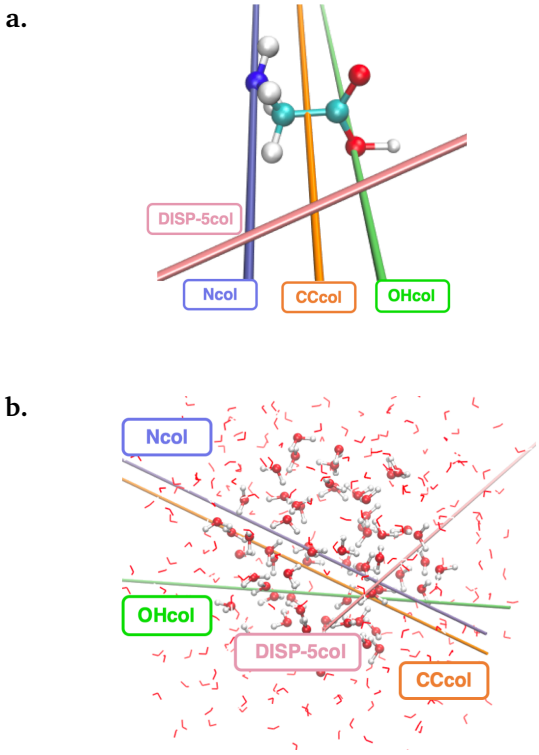

Fig. S6 H^+ collision for N-Gly and LDA isolated molecular systems. (a) H^+-N-Gly gas phase collision. All atoms treated by DFT method. Striking particle labels correspond to collisions through glycine's C-C bond (CCcol), nitrogen atom (Ncol), carboxilic oxygen (OHcol) and water molecules in the vicinity of glycine molecule (DISP-5col). (b) H^+-LDA collision. 62 atoms treated by DFT approach (ball representation) and the remaining 282 water atoms (lines representation) described by MM (TIP3P for water molecules).

D Distribution of charge migration in N-Gly-LDA system due to 1, 10 and 100keV H^+ collision

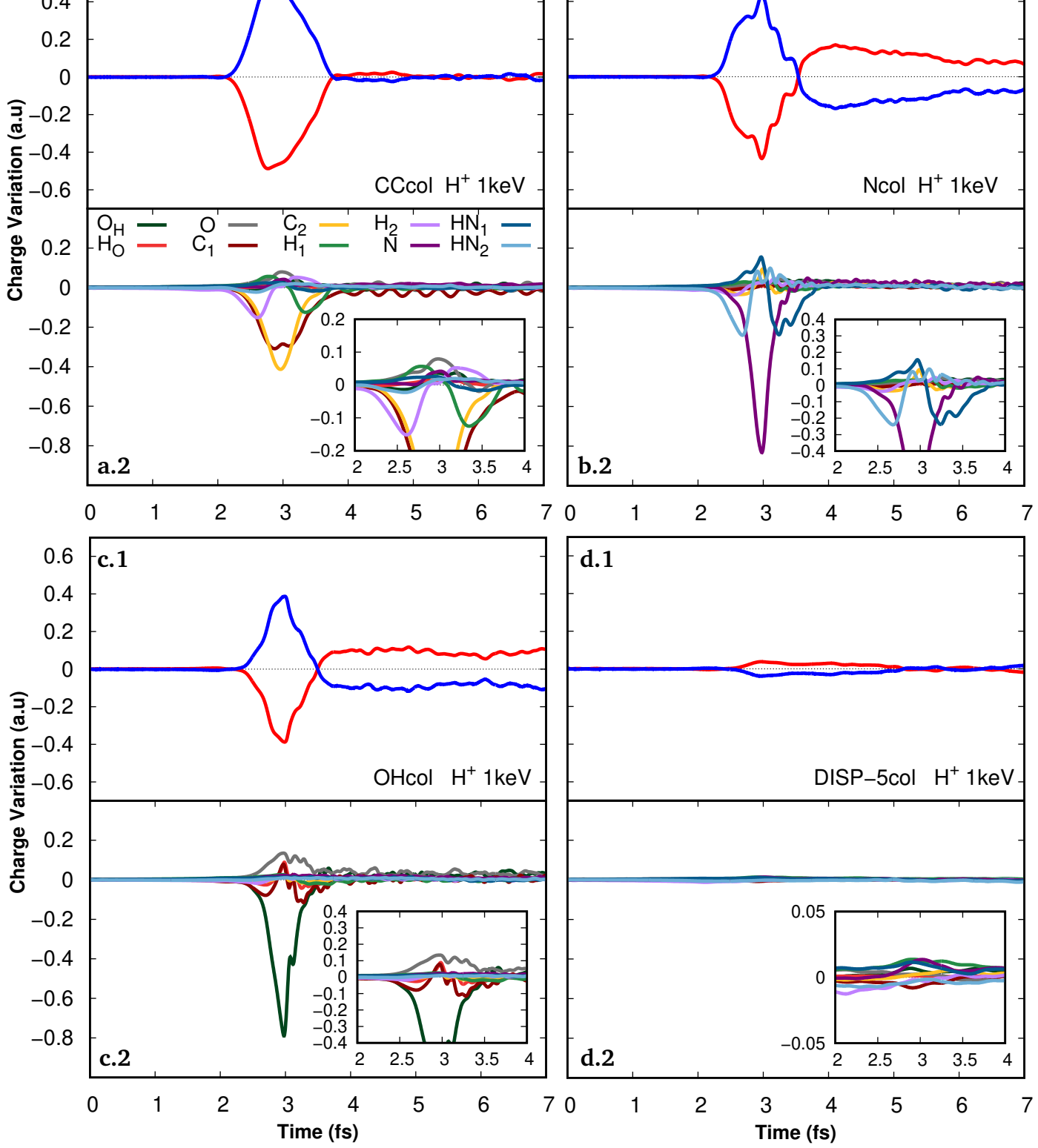

Fig. S7 Total (labeled with index 1) and N-GLY atomic charge evolution (labeled with index 2) in N-Gly-LDA molecular system under 1 keV H^+ collision with the four impact sites: (a) CCcol, (b) Ncol, (c) OHcol, and (d) DISP-5col.

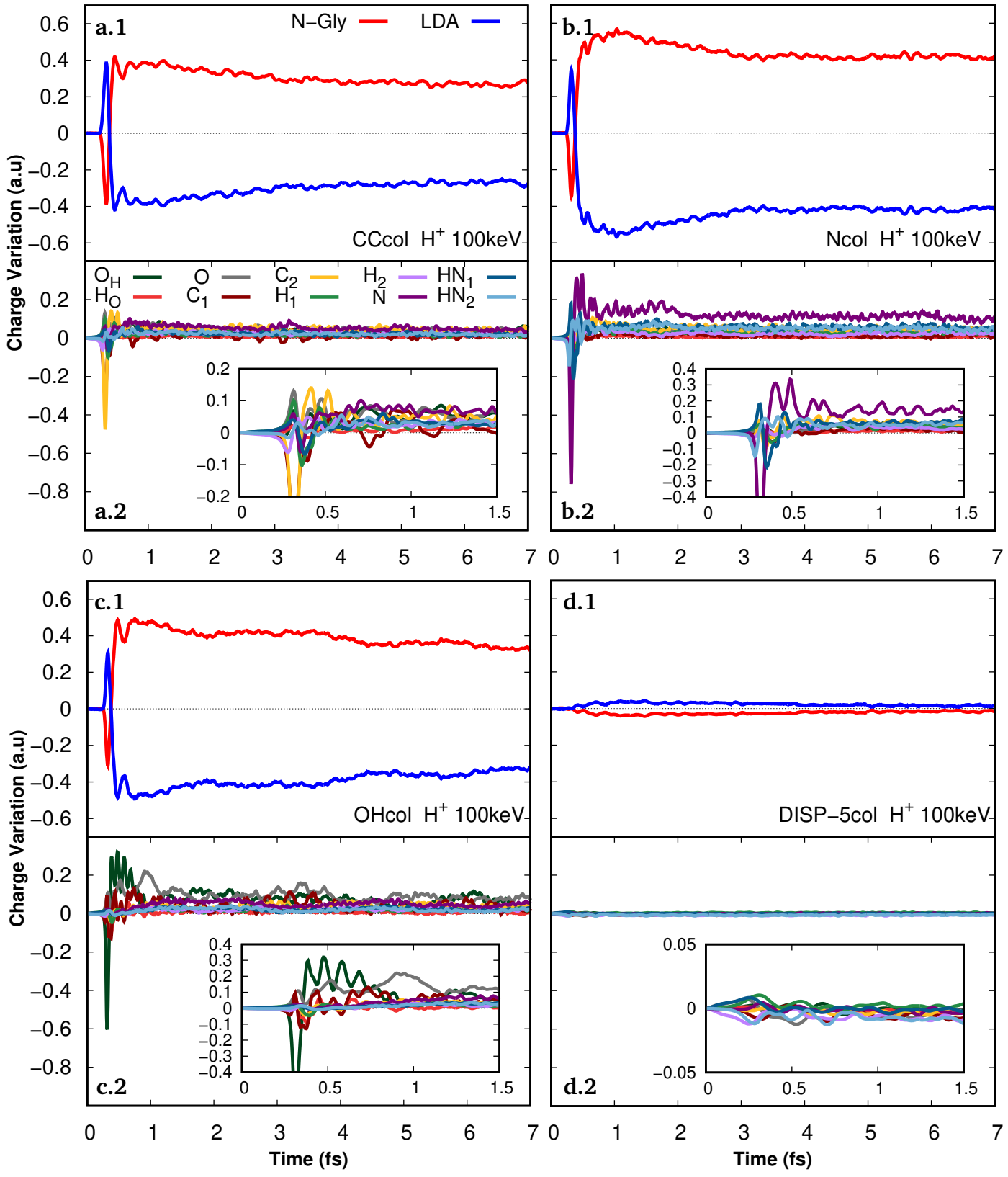

Fig. S8 Total (labeled with index 1) and N-GLY atomic charge evolution (labeled with index 2) in N-Gly-LDA molecular system under 100 keV H^+ collision with the four impact sites: (a) CCcol, (b) Ncol, (c) OHcol, and (d) DISP-5col.

Hereafter the charge variation figures for 1, 10 and 100 keV are plotted in a simpler representation. Only the charge variation curves considered to have a significant impact are shown in the graphs.

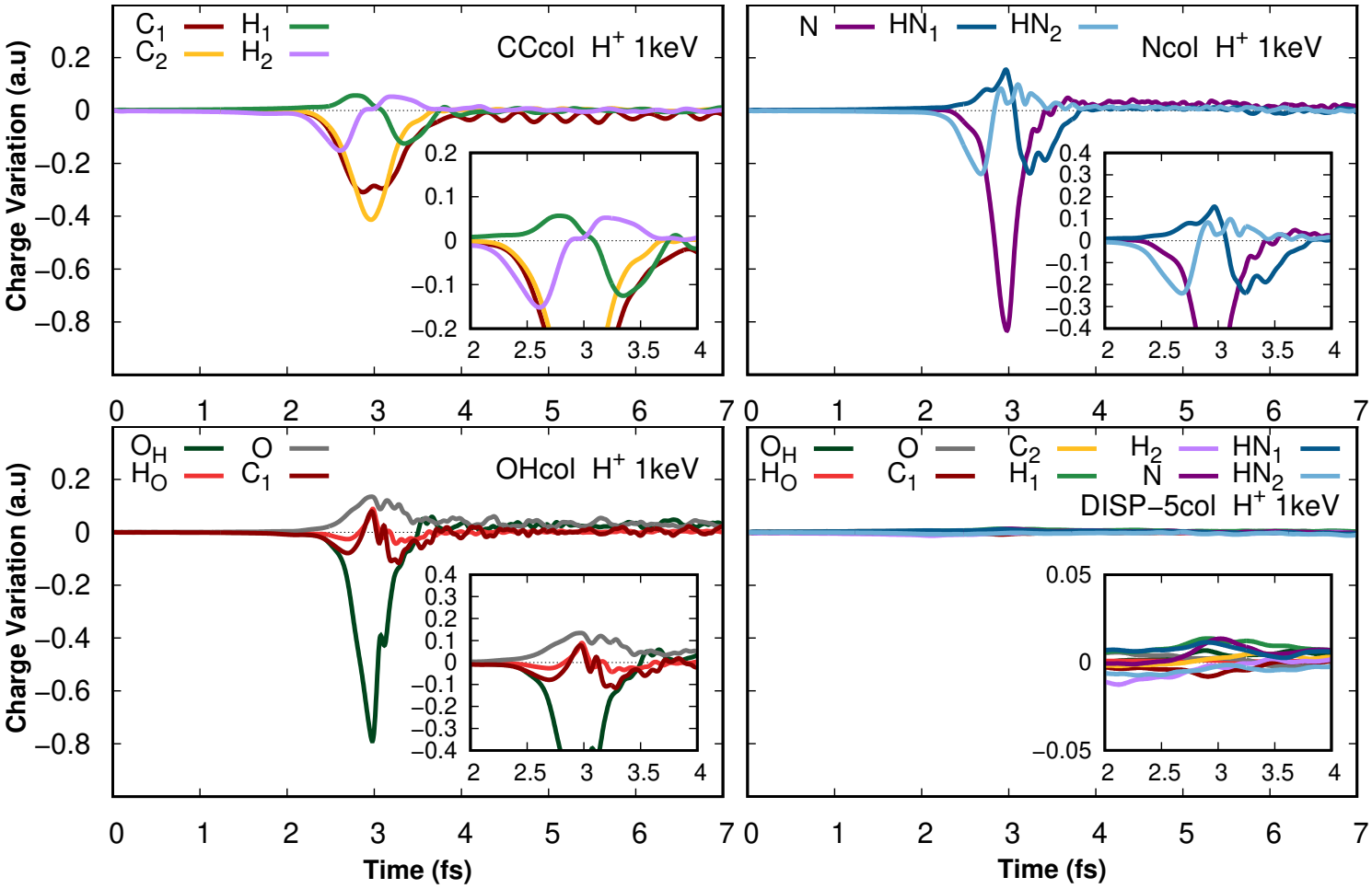

Fig. S9 N-GLY atomic charge evolution in N-Gly-LDA molecular system under 1 keV H^+ collision with the four impact sites: (a) CCcol, (b) Ncol, (c) OHcol, and (d) DISP-5col. Only curves considered to have the most significant impact in the charge variation picture are plotted.

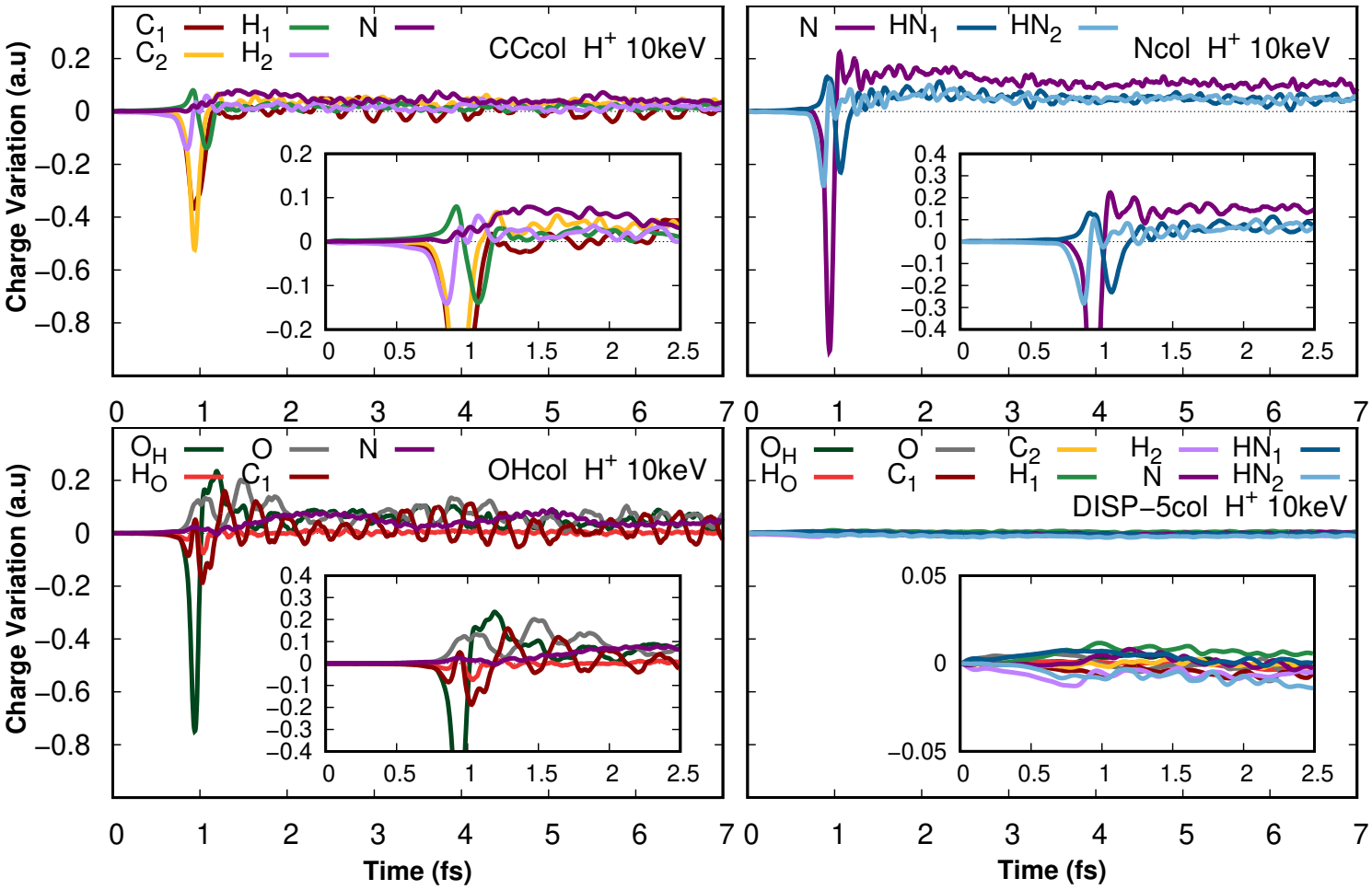

Fig. S10 N-GLY atomic charge evolution in N-Gly-LDA molecular system under 10 keV H^+ collision with the four impact sites: (a) CCcol, (b) Ncol, (c) OHcol, and (d) DISP-5col. Only curves considered to have the most significant impact in the charge variation picture are plotted.

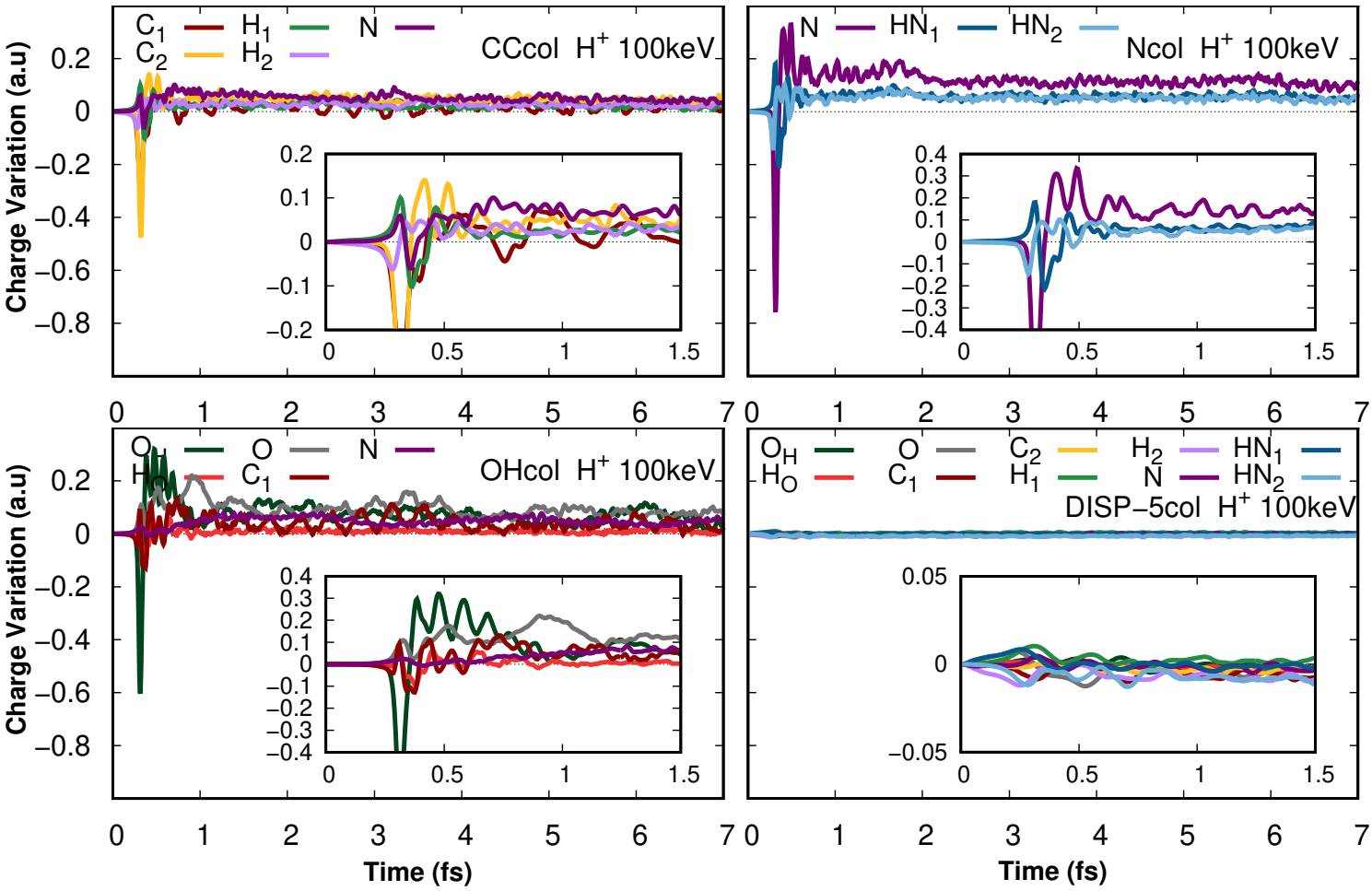

Fig. S11 N-GLY atomic charge evolution in N-Gly-LDA molecular system under 100 keV H^+ collision with the four impact sites: (a) CCcol, (b) Ncol, (c) OHcol, and (d) DISP-5col. Only curves considered to have the most significant impact in the charge variation picture are plotted.