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Supplementary Information

Dielectric Properties of Liquid Phase Molecular Clusters using External Field Method: Molecular Dynamics Study

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Chathurika D. Abeyrathne,[a,b] Malka N. Halgamuge,[b] Peter M. Farrell,[b] and Efstratios Skafidas[a,b]

[a]Centre for Neural Engineering (CfNE), [b]Department of Electrical and Electronic Engineering, The University of Melbourne, Parkville, VIC 3010, Australia.

Supplementary Information

Total Energy

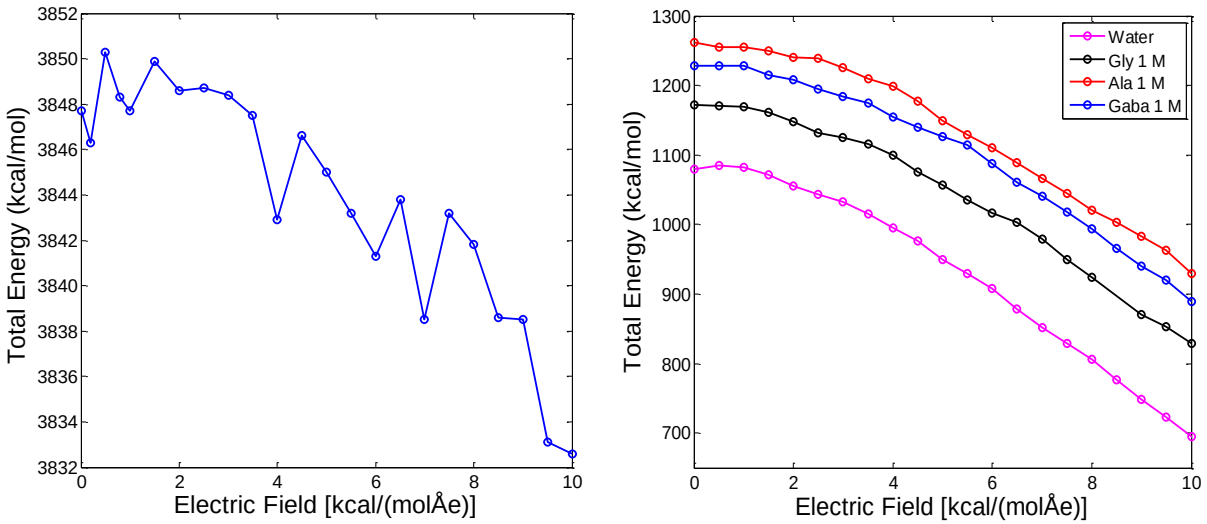

Figure S1. Variation of total energy with electric field strength, (a) 1,4-dioxane, (b) water, Gly 1 M, Ala 1 M and GABA 1 M.

The accuracy of determining the slope of the dipole moment variation curve is important for precise estimation of static dielectric constant. Thus, the energy of the system was studied as additional information. The energy of the clusters was obtained from the output of the MD simulation using VMD software. This gives the total energy of the systems, that is, the sum of potential and kinetic energies. Figure S1 shows that the total energy of 1,4-dioxane and water is constant up to 10 kcal/(molÅe) (variation is less than 1 %), and 1.5 kcal/(molÅe) (varies is less than 1%), respectively, whereas that of 1 M of bio-molecular aqueous solutions is constant up to 1.0 kcal/(molÅe) (varies is less than 1%). Thus, the slope of Fig. 1, 2 and 3 was obtained by fitting <Mz> up to linear equation where the variation of total energy is less than 1%.

Radial Distribution Function

The structural changes of molecular clusters in the presence of external electric fields can be obtained using the radial distribution function (RDF). The RDF was obtained from the trajectory file generated from the MD simulations using VMD software. The changes in RDFs of 1,4-dioxane and water are hardly outside the limits of statistical uncertainty for the field strengths concerned in this study, indicating that there are no structural changes up to electric fields of 10 kcal/(molÅe) (4.334×10^7 V/cm).

The structural changes of Gly 1 M are negligible, whereas small changes can be seen in Ala 1 M and considerable changes in GABA 1 M are observed. The structural changes of Ala 1 M and GABA 1 M due to external electric fields are shown in Fig. S2 - S5. In these figures, nitrogen$^+$–water, and nitrogen$^+$-oxygen$^-$ RDFs of

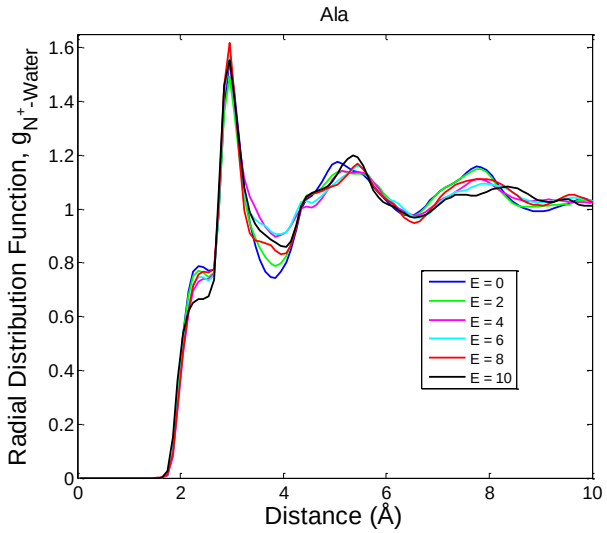

Figure S2. Radial distribution functions between N^+ of alanine and water (N^+-Water) for different electric fields. The unit of field strength (*E*) is kcal/(molÅe).

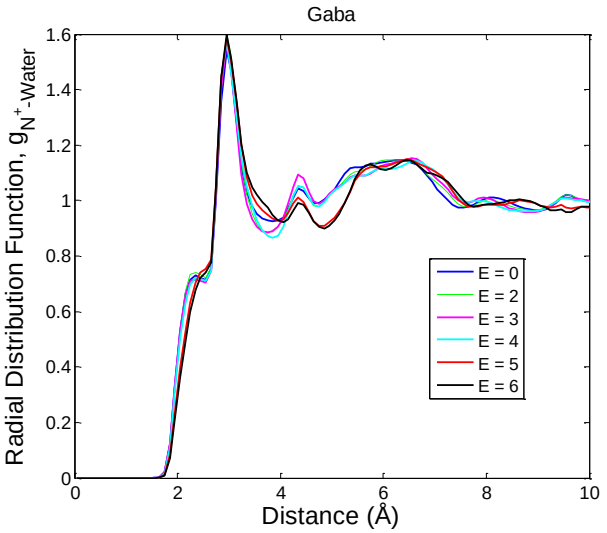

Figure S4. Radial distribution functions between N^+ of GABA and water (N^+-Water) for different electric fields. The unit of field strength (*E*) is kcal/(molÅe).

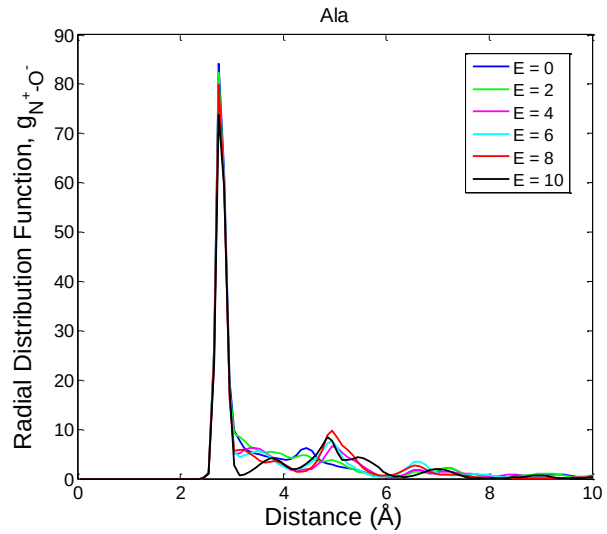

Figure S3. Radial distribution functions between N^+ and O^- of alanine (N^+-O^-) for different electric fields. The unit of field strength (*E*) is kcal/(molÅe).

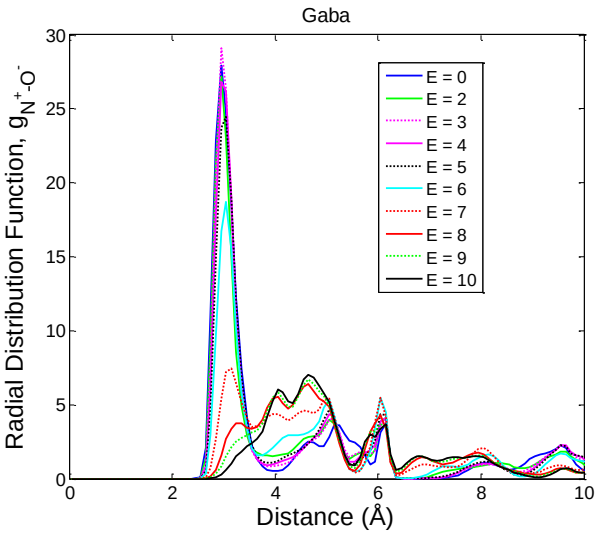

Figure S5. Radial distribution functions between N^+ and O^- of GABA (N^+-O^-) for different electric fields. The unit of field strength (*E*) is kcal/(molÅe).

alanine and GABA are presented. They can be considered to reflect the structural changes of pure water, alanine and GABA caused by external electric fields of various strengths. The electric fields affect the structure of alanine and water, as shown in Fig. S2 - S3. The RDF of nitrogen$^+$- water of alanine shows a small change in the height of first minima indicating the broadening of first peak, though the positions of the first peaks are not affected by the application of an external field. Thus the density of water shows small changes in the presence of alanine due to external electric fields. Figure S3 illustrates that the height of first peak of nitrogen$^+$-oxygen$^-$ RDF decreases where a considerable difference (12 %) can be seen at 10 kcal/(molÅe) (4.334×10^7 V/cm).

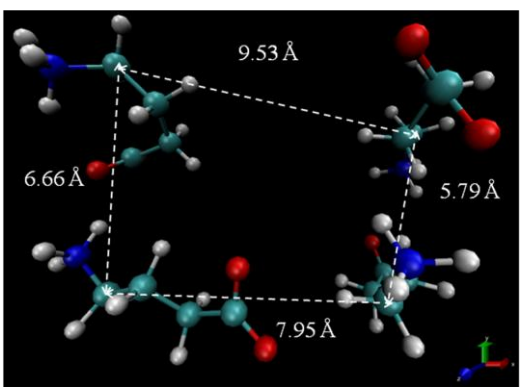

Figure S6. Orientation of GABA molecules when there is no external electric field.

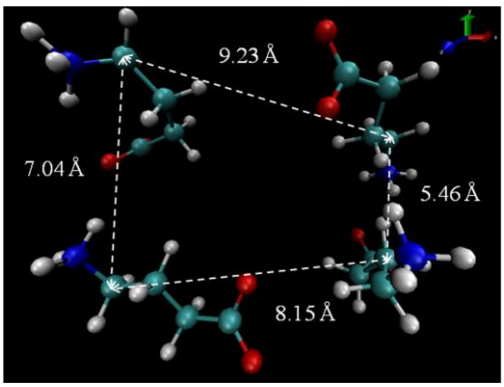

Figure S7. Orientation of GABA molecules when the external electric field is 6 kcal/(molÅe).

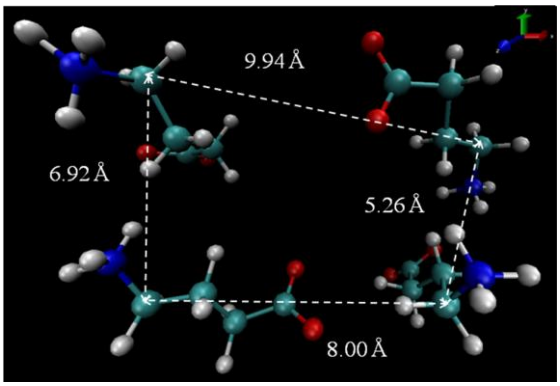

Figure S8. Orientation of GABA molecules when the external electric field is 10 kcal/(molÅe).

The density of water molecules changes in the presence of GABA more than in the presence of alanine (Fig. S4). There is a large change in the RDF of nitrogen^{+}-oxygen^{-} of GABA after 5 kcal/(molÅe) (2.167×10^{7} V/cm) as shown in Fig. S5. The height of first peak decreases and shifts with increasing field strength. The rotation of the GABA molecules caused by the external electrical field is shown in Fig. S6 - S8.