Electronic Supplementary Information

Molecular dynamics simulations of aqueous glycine solutions

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**Fig. S1.** Typical energy and volume fluctuations during the productive run.
### Table S1. Duration of Simulations, ns

<table>
<thead>
<tr>
<th>T=300 K, Charge set</th>
<th>Number of glycine molecules in solution</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>N=12</td>
<td>N=36</td>
</tr>
<tr>
<td>CNDO</td>
<td>3.8</td>
<td>3.5</td>
</tr>
<tr>
<td>B3LYP</td>
<td>3.0</td>
<td>3.1</td>
</tr>
<tr>
<td>mB3LYP</td>
<td>3.4</td>
<td>3.0</td>
</tr>
</tbody>
</table>

### Duration, ns (mB3LYP, N=72)

<table>
<thead>
<tr>
<th>Electric field</th>
<th>T=300 K</th>
<th>T=350 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>E=0 V/m</td>
<td>3.4</td>
<td>3.3</td>
</tr>
<tr>
<td>E=10³ V/m</td>
<td>4.0</td>
<td>3.3</td>
</tr>
<tr>
<td>E=10⁴ V/m</td>
<td>4.3</td>
<td>5.3</td>
</tr>
</tbody>
</table>
Calculation of Diffusion Coefficients

**Start time 200 ps**

**GLYCINE**

\[ m = 0.56 \]

**WATER**

\[ m = 0.56 \]

**Start time 300 ps**

**GLYCINE**

\[ m = 0.56 \]

**WATER**

\[ m = 0.56 \]

**Start time 400 ps**

**GLYCINE**

\[ m = 0.56 \]

**WATER**

\[ m = 0.56 \]
Mean Standard Deviation SE of mean Lower 95% CI of Mean Upper 95% CI of Mean
1.1865 0.12408 0.06204 0.98907 1.38393
2.5135 0.07636 0.03818 2.392 2.635

**Fig. S2.** Mean square displacement of glycine and water molecules during 100 ps time intervals on 0.5 ns trajectory due to diffusion at $m=0.56$ mol/kg
Fig. S3. Mean square displacement of glycine and water molecules during 100 ps time intervals due to diffusion at $m=3.33$ mol/kg.
Fig. S4 Radial distribution functions, $g_{NO}(r)$, and running coordination numbers, $N_{NO}(r)$, for nitrogens and oxygens of glycine in aqueous solutions with various solute concentrations, $m$. 

\[ m = 3.33 \text{ mol/kg} \]
\[ m = 1.57 \]
\[ m = 0.55 \]
**Fig. S5.** Glycine clusters consisting from 15 glycine molecules, nitrogen atoms are presented by yellow balls. Sticks connect the nearest nitrogens.
Fig. S6. Snapshots of the simulation box at $m=3.33$ mol/kg. Nitrogen atoms are presented by yellow balls. Sticks connect the nearest nitrogens. Water molecules are not shown for clarity. Time interval between snapshots is equal to 10 ps.
Fig. S7. Small glycine clusters in aqueous solution at $m=3.33$ mol/kg

Fig. S8. Average cosine of the angle between vectors connecting carbon atoms (H$_2$C→CO$_2$) in two glycine molecules calculated without and with dc electric field ($E=10^3$ and $10^4$ V/m) applied to solution at $m=3.33$ mol/kg ($T=300$ K and $350$ K)

Fig. S9. (a) Crystallographic unit cell of $\gamma$-glycine, (b) $2\times2\times2$ unit cells.
**Fig. S10.** Number of glycine clusters, $n_s$, in the saturated aqueous solution as a function of cluster size, $s$: (a) for small clusters, (b) for other clusters.

**Fig. S11.** Number of glycine clusters, $n_s$, in the saturated aqueous solution as a function of cluster size, $s$: (a) for small clusters, (b) for all clusters. The mB3LYP force field is used. Data calculated at 300 K and 350 K for solutions in the electric field and without the electric field are presented.
Fig. S12. Glycine clusters observed in aqueous solutions at $m=3.33$ mol/kg and $E=10^4$ V/m. (a) stripe-like clusters; (b) chain-like and stripe-like clusters, sticks connect the nearest nitrogens ($r_{NN}<6$ Å), water molecules and monomers are not shown for clarity.
Fig. S13. Radius of gyration, $R_g$, of glycine clusters in the saturated aqueous solution as a function of cluster size, $s$.

Fig. S14. Radius of gyration, $R_g$, of glycine clusters in the saturated aqueous solution as a function of cluster size, $s$: (a) for small clusters, (b) for all clusters. The mB3LYP force field is used. Data calculated at 300 K and 350 K for solutions in the electric field and without the electric field are presented.
**Fig. S15.** Radial distribution functions, \( g(r) \), of water oxygens with respect to nitrogens (NOw) and carbons of \(-\text{COO}\) groups (COw).

**Fig. S16.** Fractions of water molecules from the first hydration shells of \(-\text{NH}_3\) groups vs. lifetimes.
Fig. S17. Fractions of glycine molecules vs. lifetimes.