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

Effect of spacer chain length on the liquid structure of aqueous dicationic ionic liquid solutions: Molecular dynamics studies

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Supplementary Information

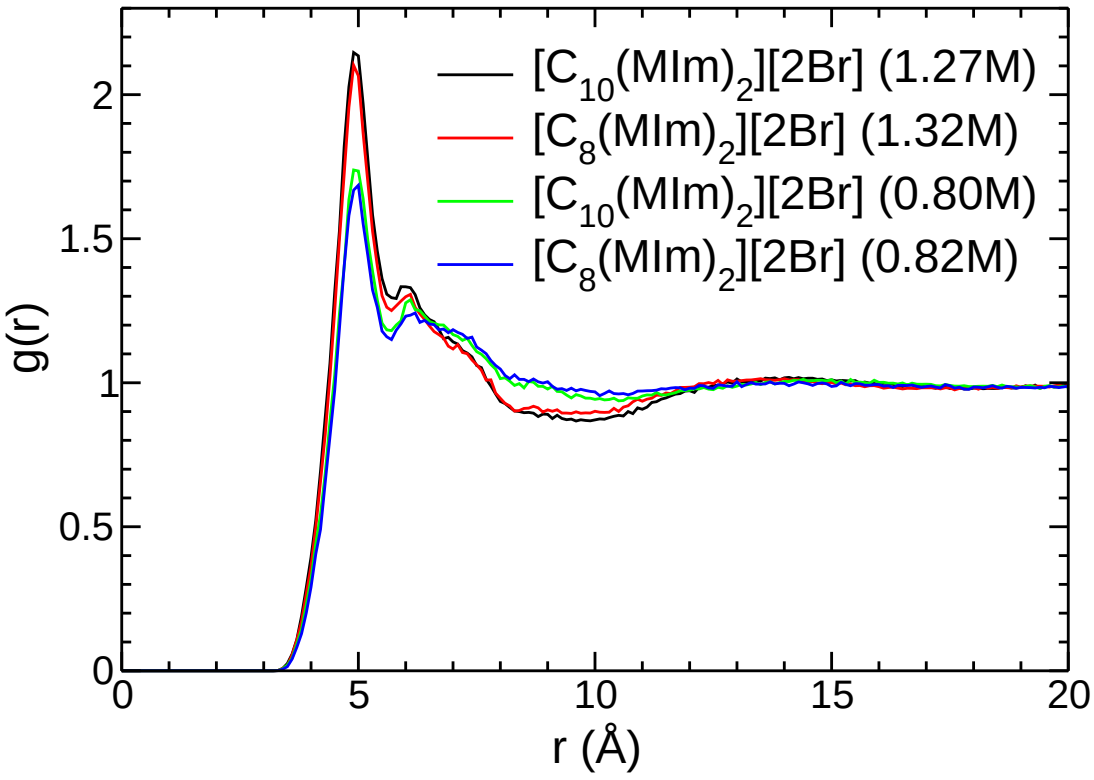

Figure S1: RDFs of anions around the geometric center of the imidazolium rings in aqueous solutions

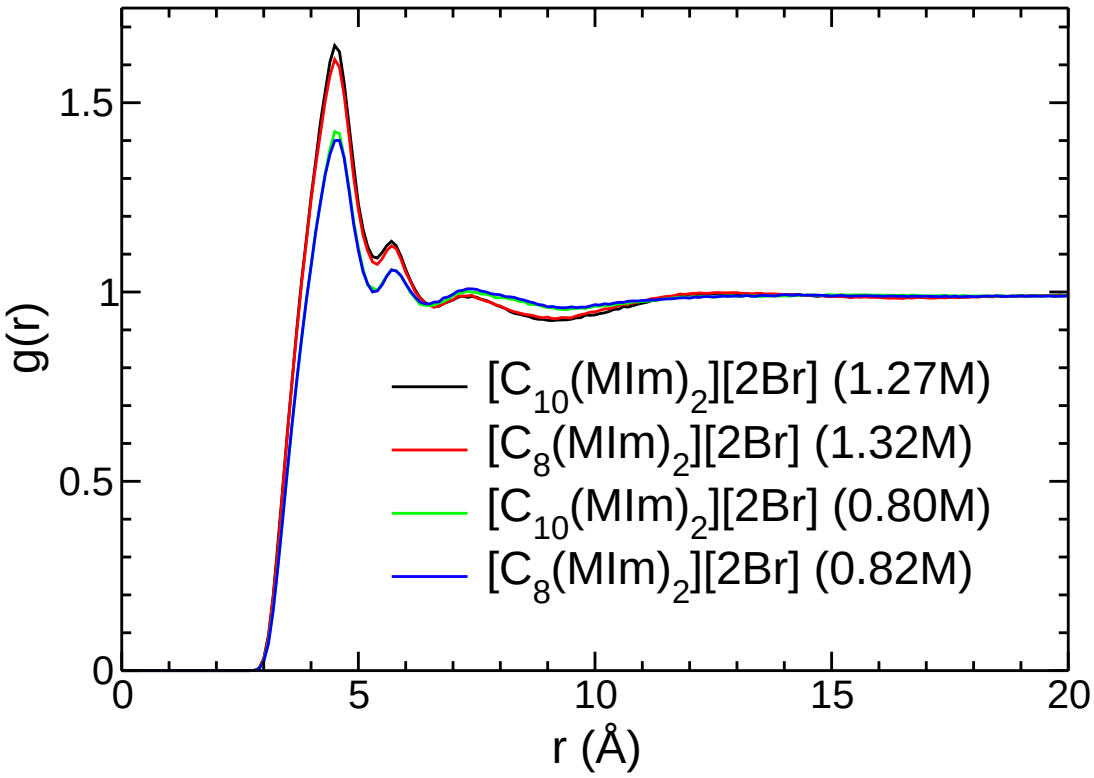

Figure S2: RDFs of water molecules around the geometric center of the imidazolium rings in aqueous solutions

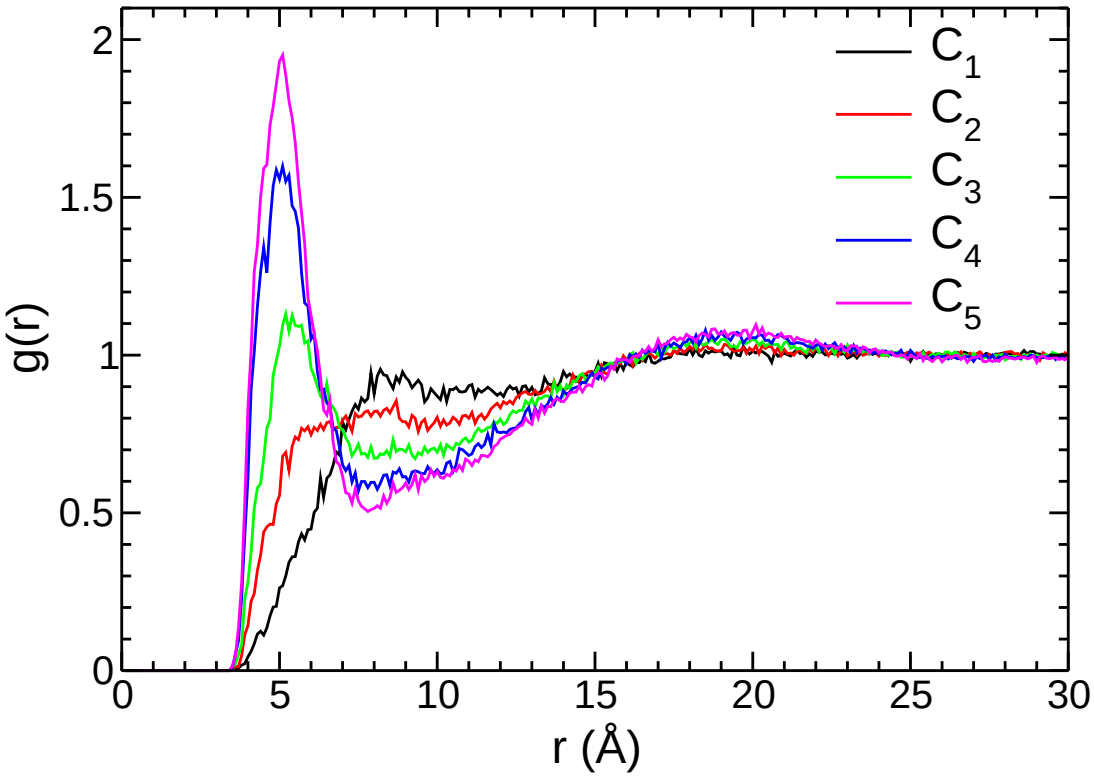

Figure S3: RDFs of different carbon atoms of the decyl spacer around themselves in aqueous solution of $[C_{10}(MIm)_2][2Br]$.

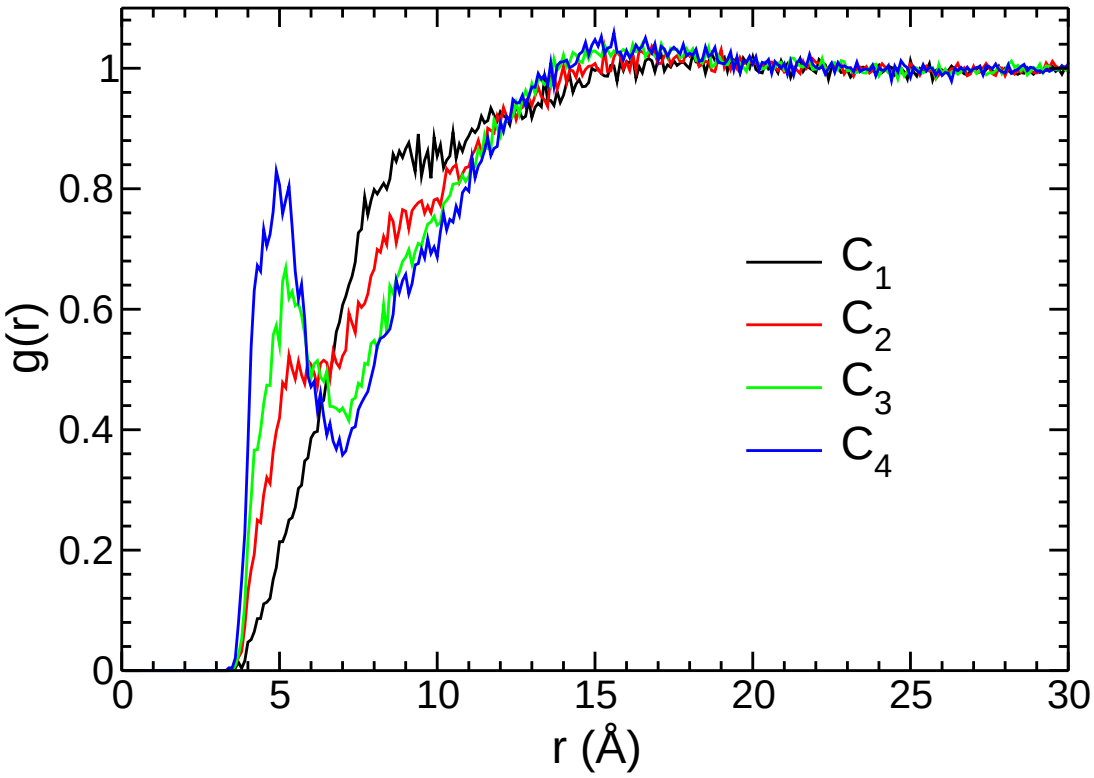

Figure S4: RDFs of different carbon atoms of the octyl spacer around themselves in aqueous solution of $[C_8(MIm)_2][2Br]$.

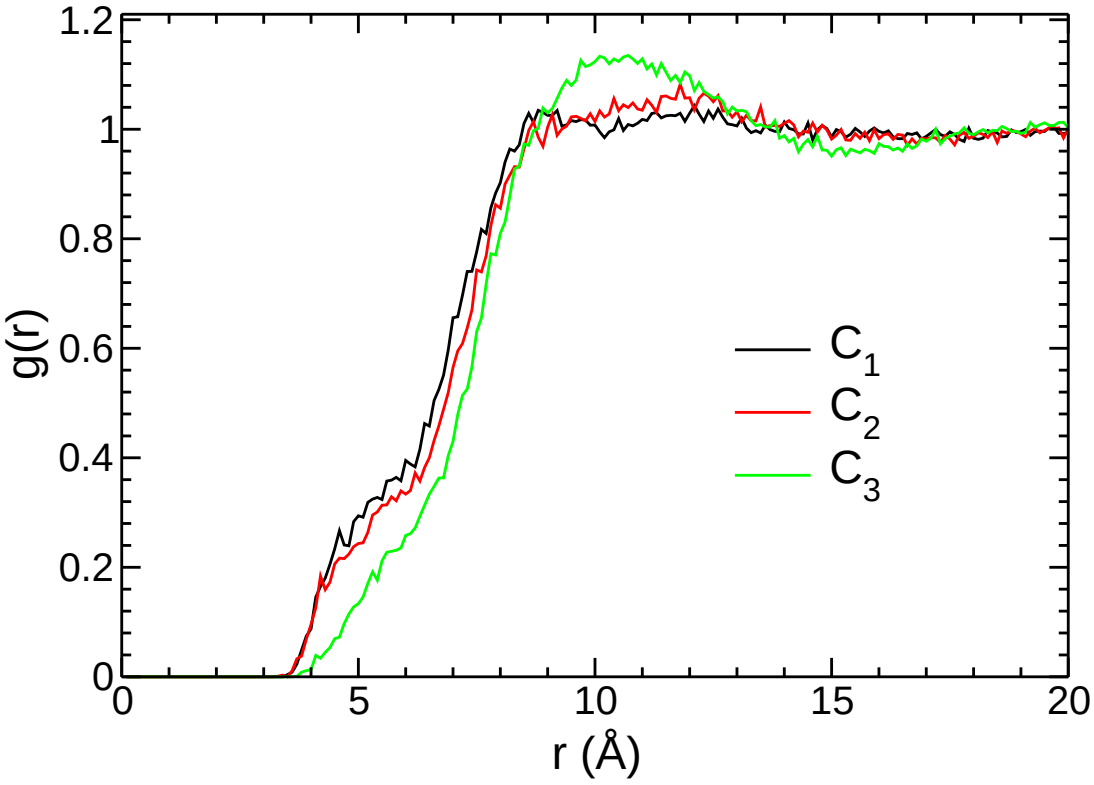

Figure S5: RDFs of different carbon atoms of the pentyl spacer around themselves in aqueous solution of $[C_5(MIm)_2][2Br]$.

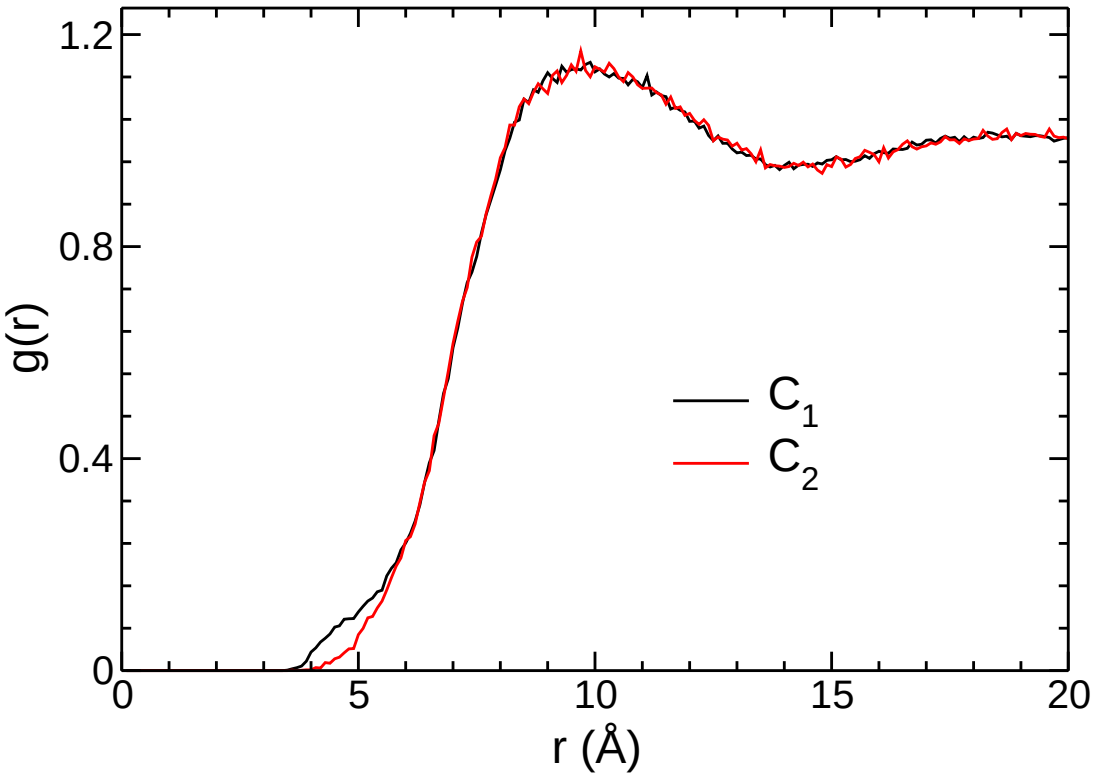

Figure S6: RDFs of different carbon atoms of the propyl spacer around themselves in aqueous solution of [C_3(MIm)$_2$][2Br].

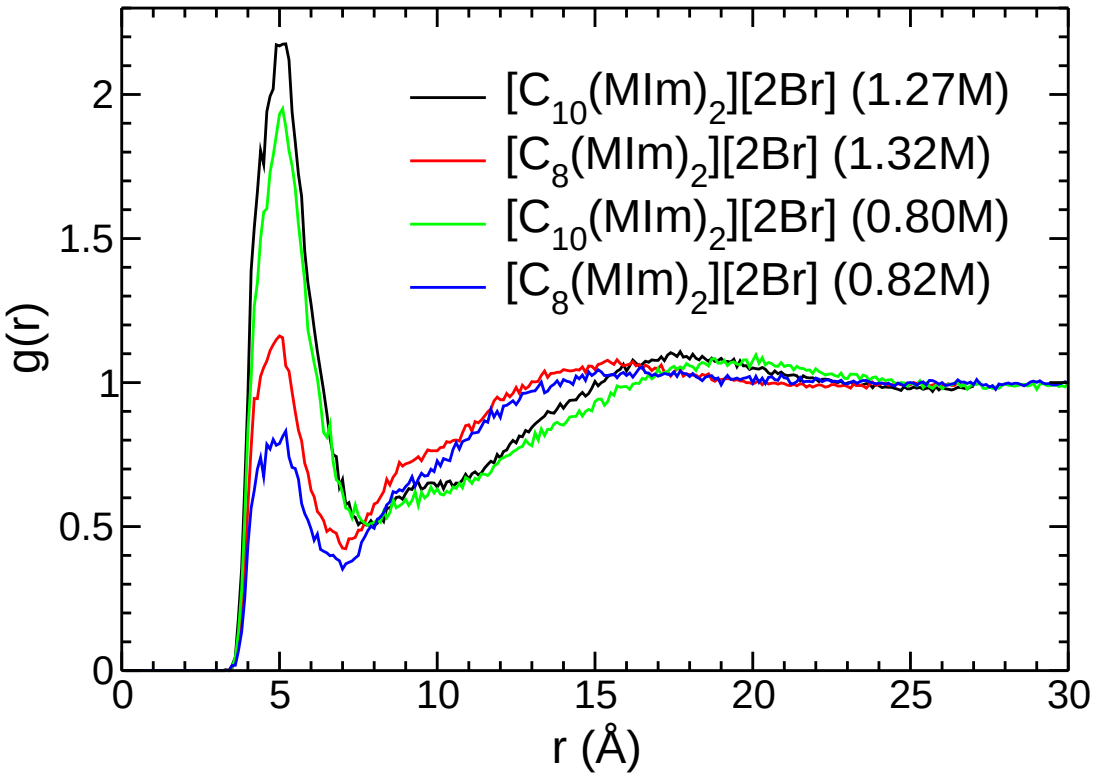

Figure S7: RDFs of central carbon atom of the spacer chain around themselves in aqueous solutions of $[C_{10}(MIm)_2][2Br]$ and $[C_8(MIm)_2][2Br]$.

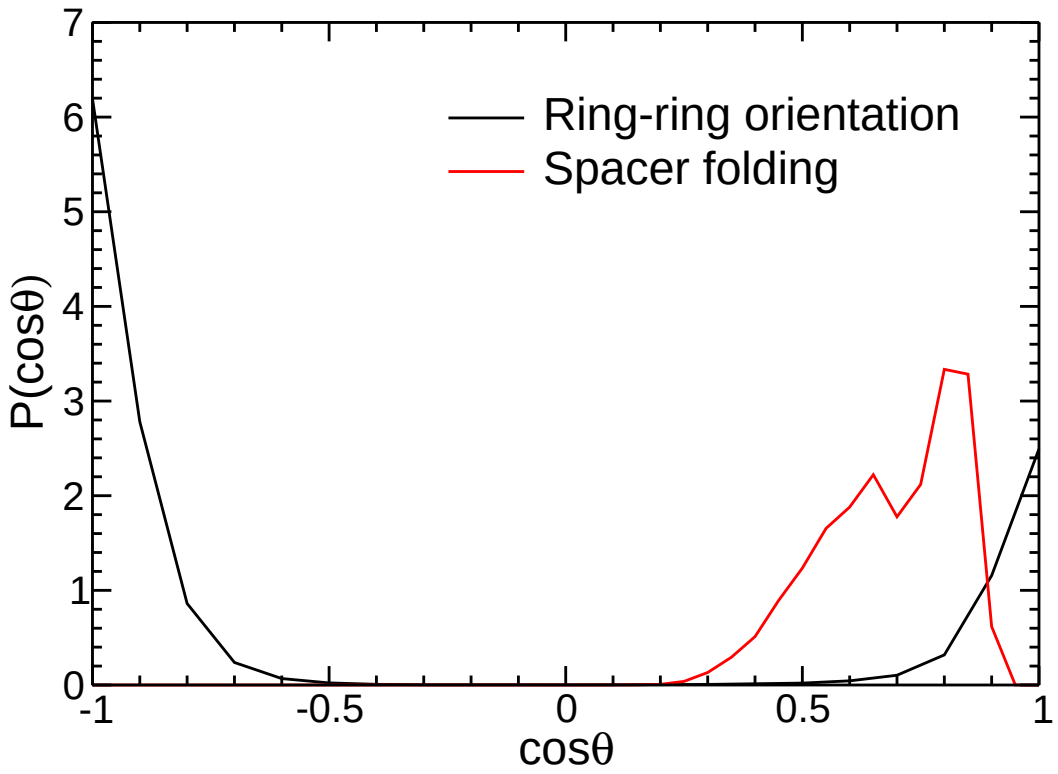

Figure S8: Distribution of angles between the normal vectors of two imidazolium rings, and two vectors joining the central carbon atom of the spacer with the imidazolium nitrogen atoms connected to the spacer in $[C_{16}(MIm)_2][2Br]$ in gas phase.

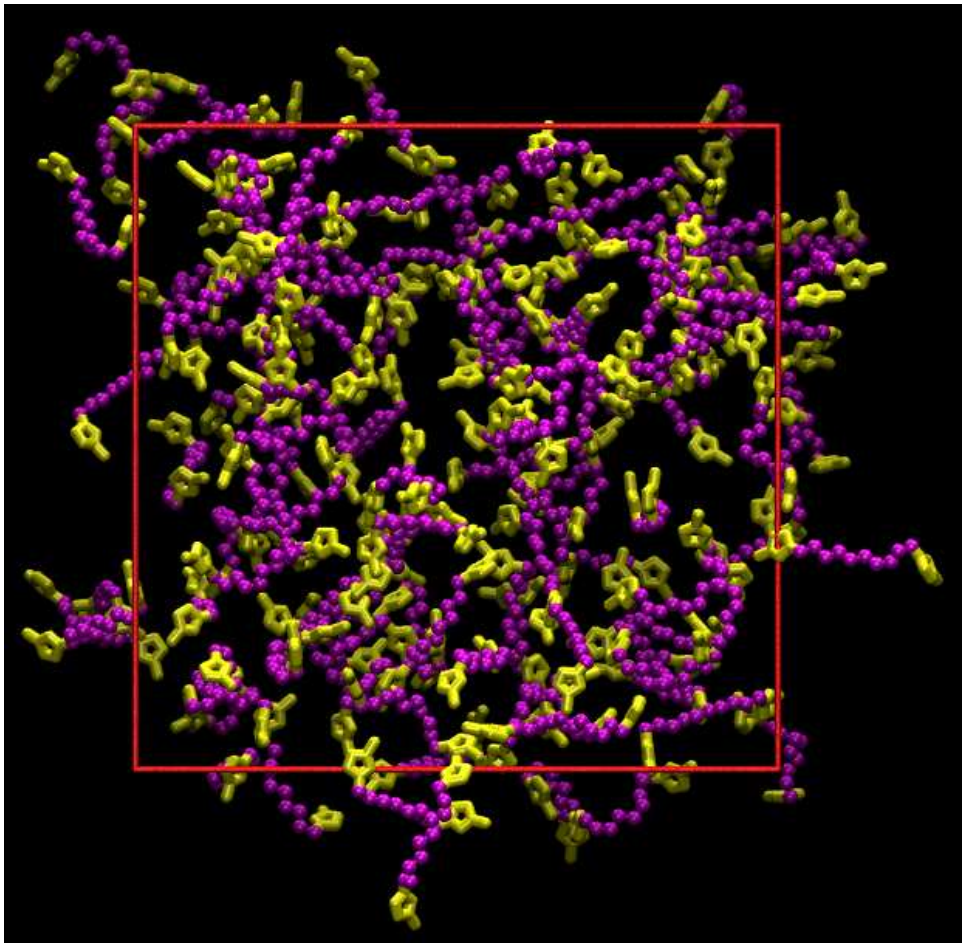

Figure S9: Snapshot of the aqueous solution of $[C_{10}(MIm)_2][2Br]$ after 50 ns simulation. Head groups are shown in yellow and the tail groups are shown in magenta. Anions, water and hydrogen atoms on the cation are not shown for the ease of visualization.

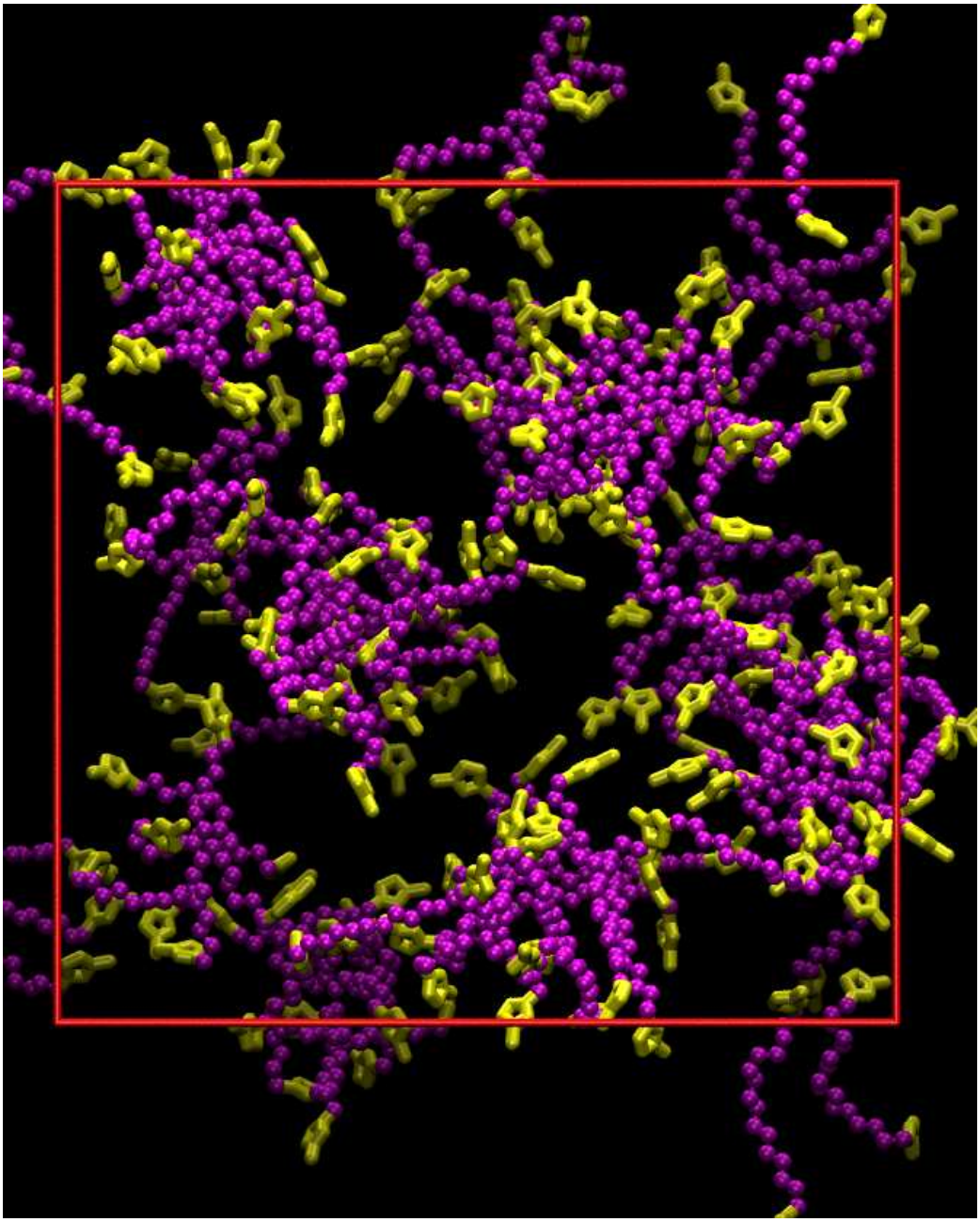

Figure S10: Snapshot of the aqueous solution of $[C_{16}(MIm)_2][2Br]$ after 50 ns simulations. Head groups are shown in yellow and the tail groups are shown in magenta. Anions, water and hydrogen atoms on the cation are not shown for the ease of visualization.

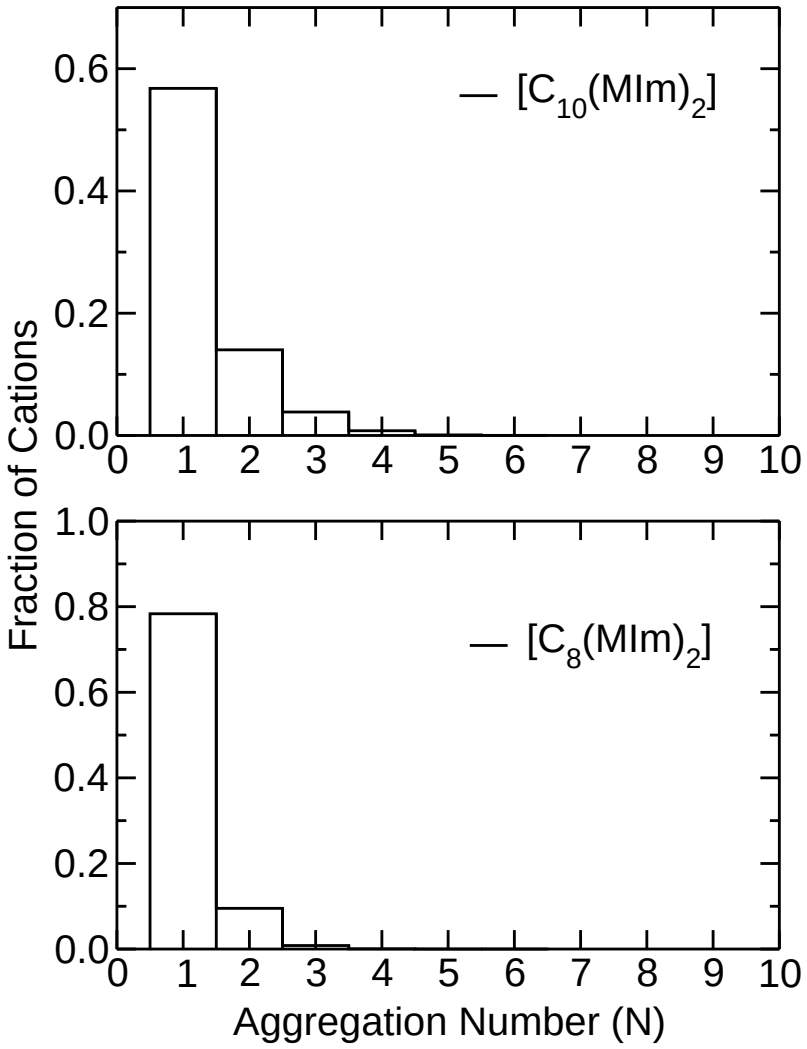

Figure S11: Fraction of cations involved in forming aggregates of size N in aqueous solutions of $[C_{10}(MIm)_2][2Br]$ and $[C_8(MIm)_2][2Br]$.

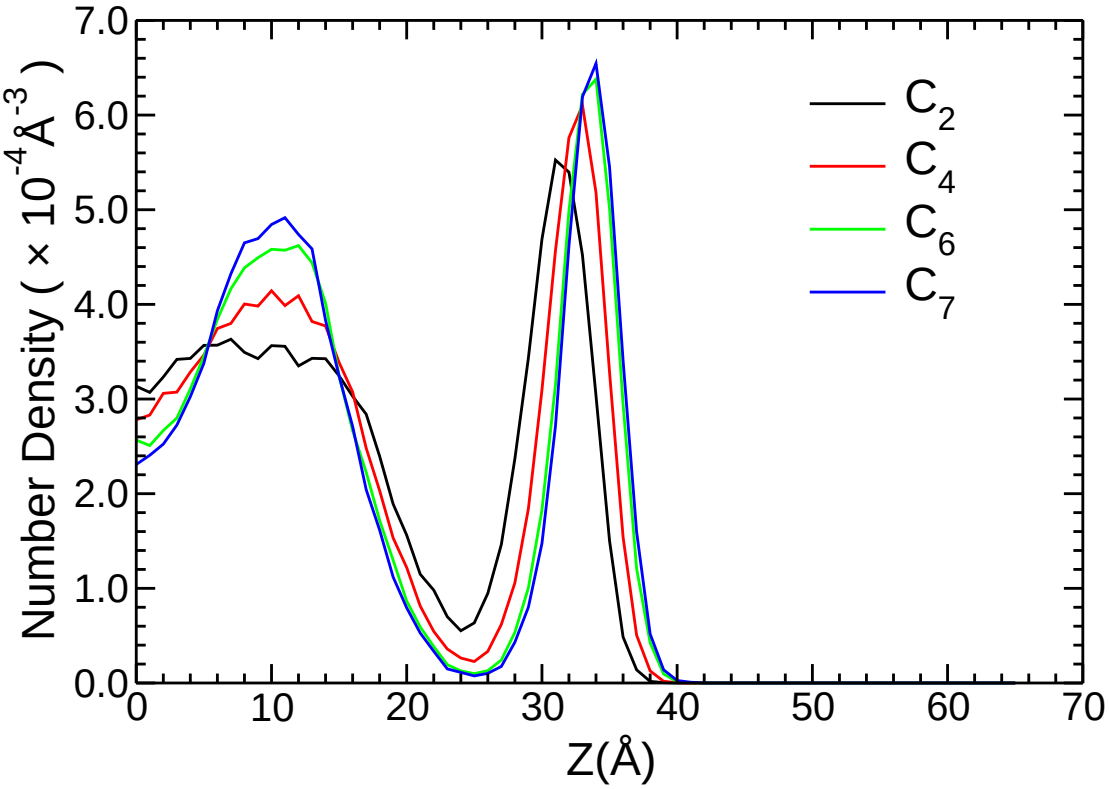

Figure S12: Atom number density profiles of different carbon atoms of the hexadecyl spacer along the interface normal (z-axis) in the liquid–vapor interface of [C_{16}(MIm)$_2$][2Br] solution.

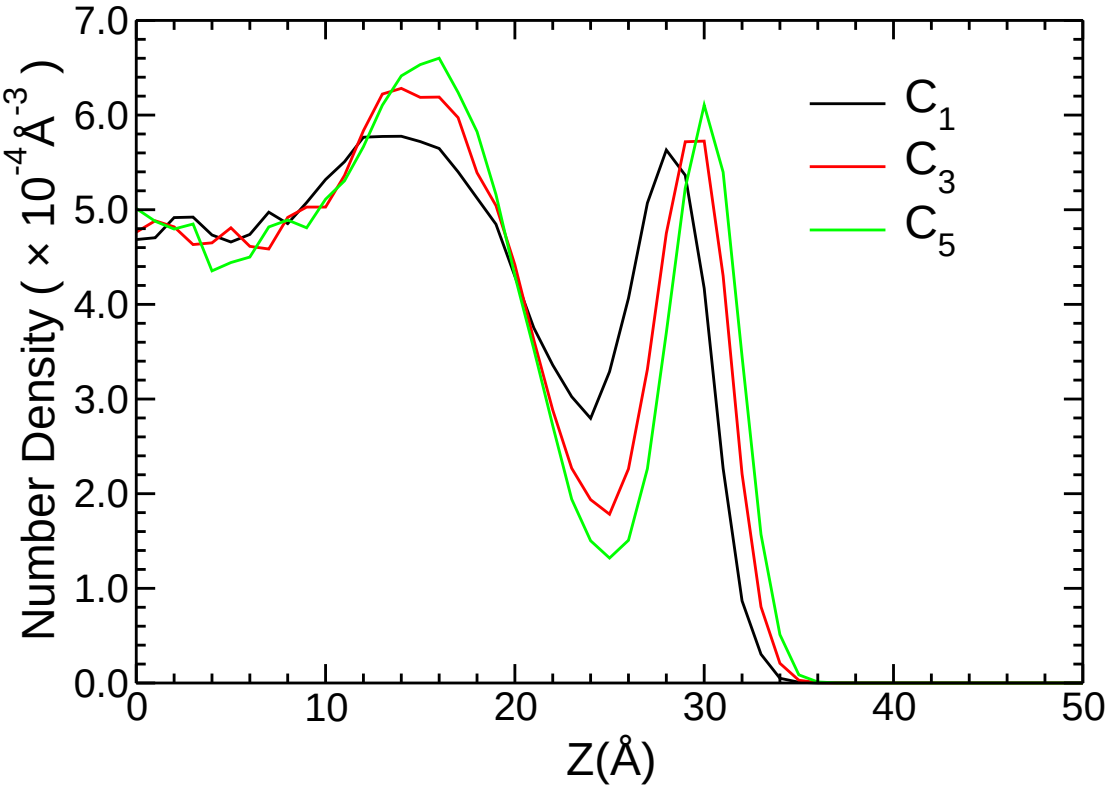

Figure S13: Atom number density profiles of different carbon atoms of the decyl spacer along the interface normal (z-axis) in the liquid–vapor interface of $[C_{10}(MIm)_2][2Br]$ solution.

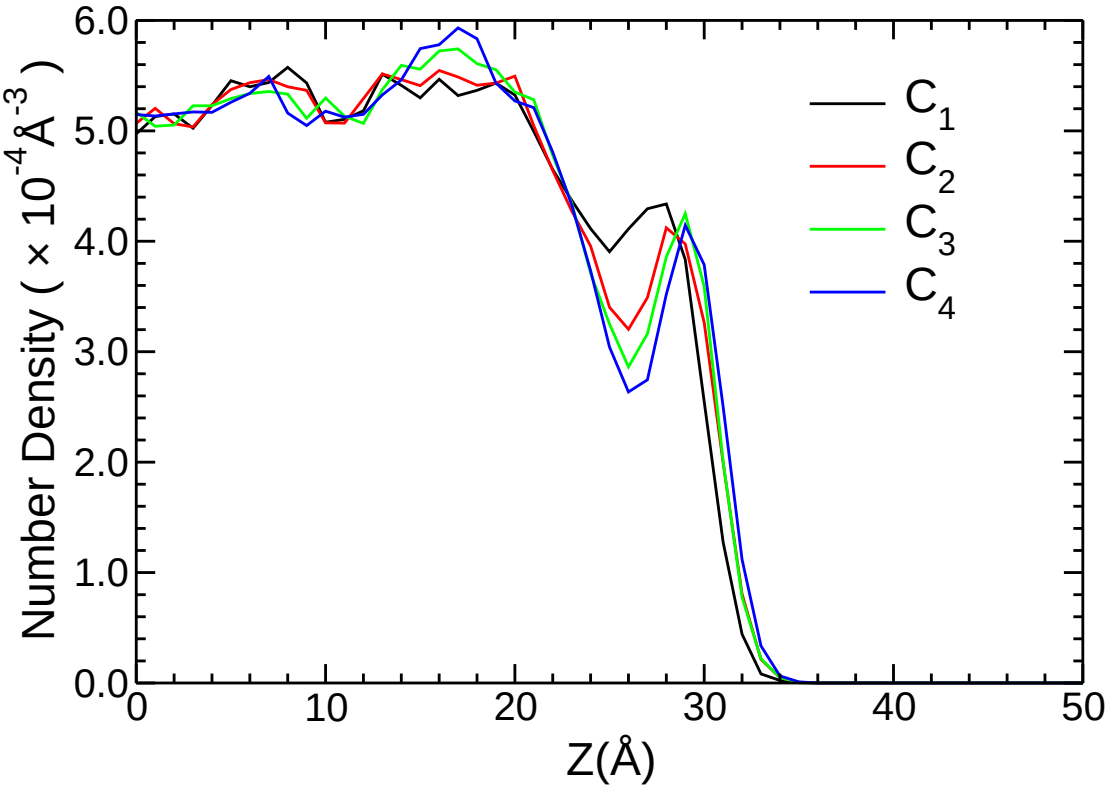

Figure S14: Atom number density profiles of different carbon atoms of the octyl spacer along the interface normal (z-axis) in the liquid–vapor interface of $[C_8(MIm)_2][2Br]$ solution.

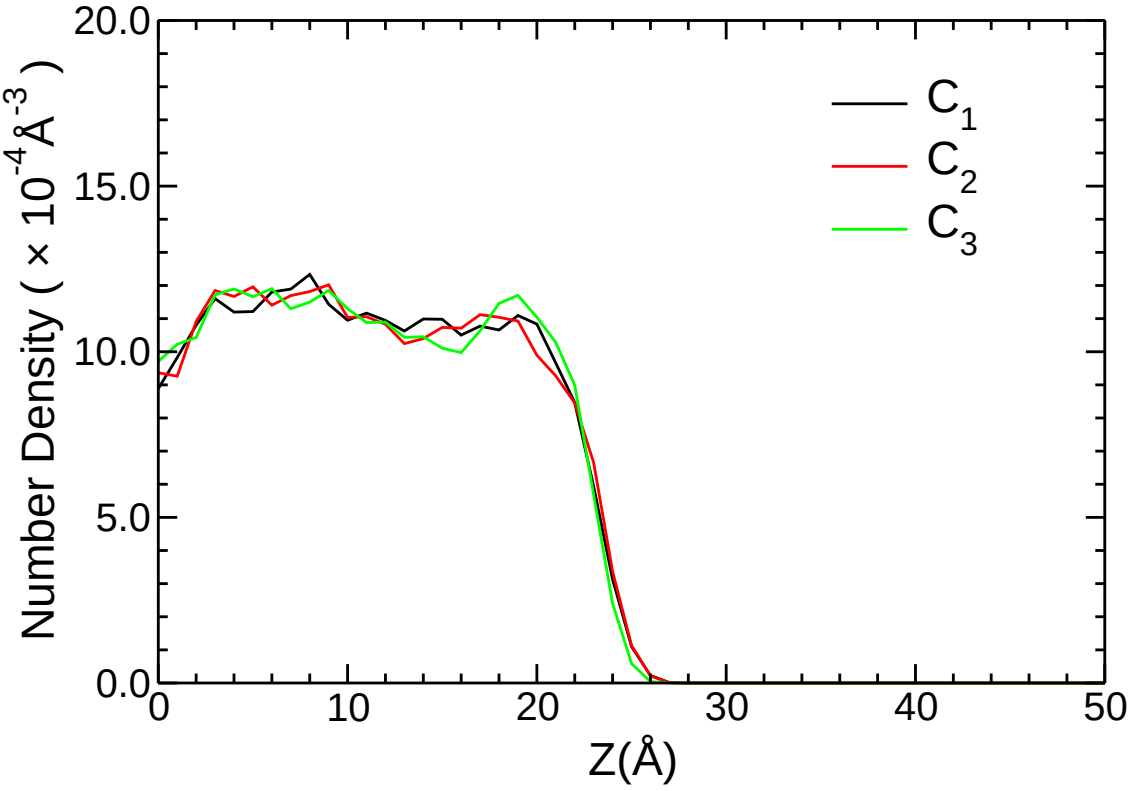

Figure S15: Atom number density profiles of different carbon atoms of the pentyl spacer along the interface normal (z-axis) for the $[C_5(MIm)_2]$ cations in aqueous solution.

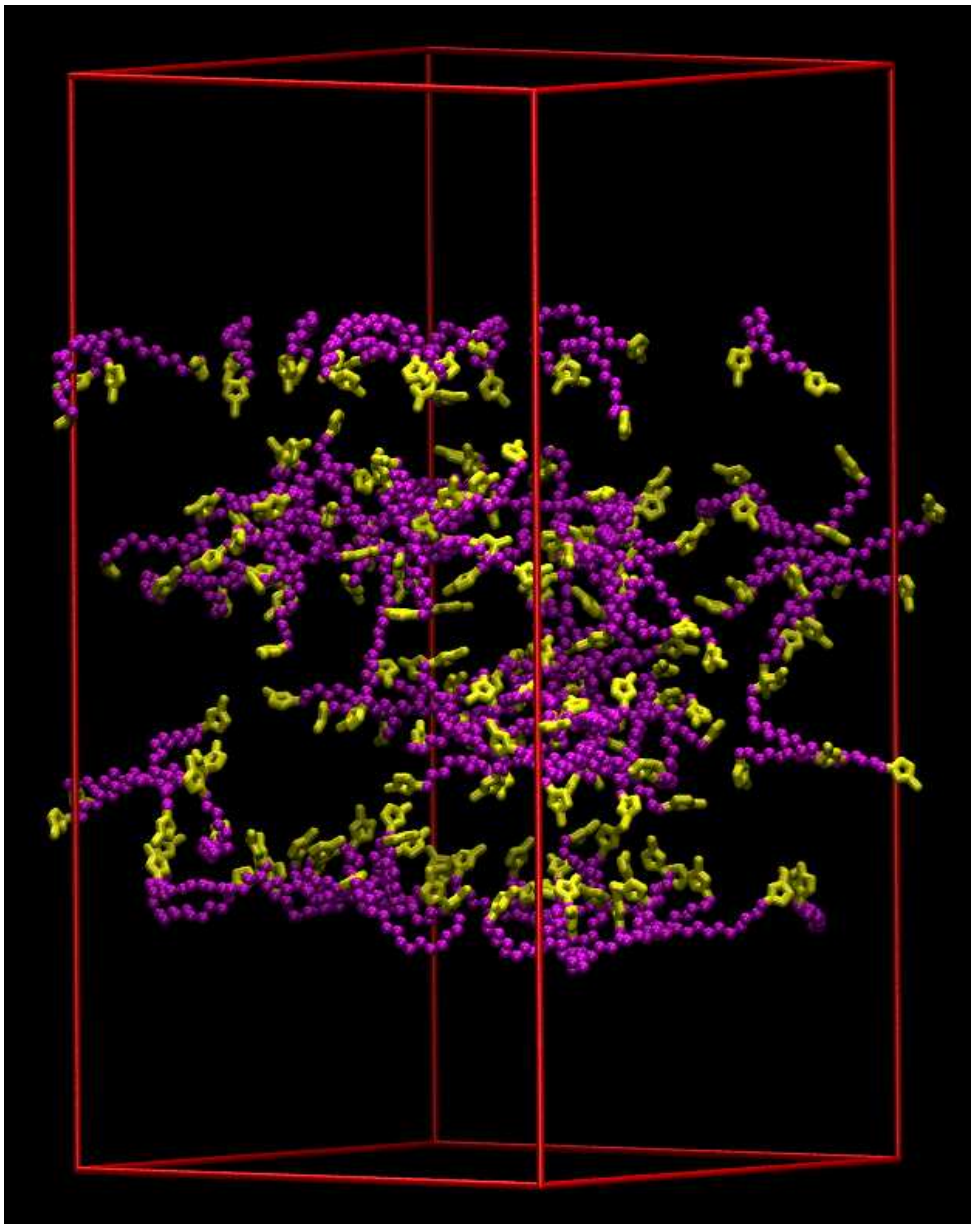

Figure S16: Snapshot of the liquid–vapor interface of the aqueous solution of $[C_{16}(MIm)_2][2Br]$ after 25 ns simulations. Head groups are shown in yellow and the tail groups are shown in magenta. Anions, water and hydrogen atoms on the cation are not shown for the ease of visualization.

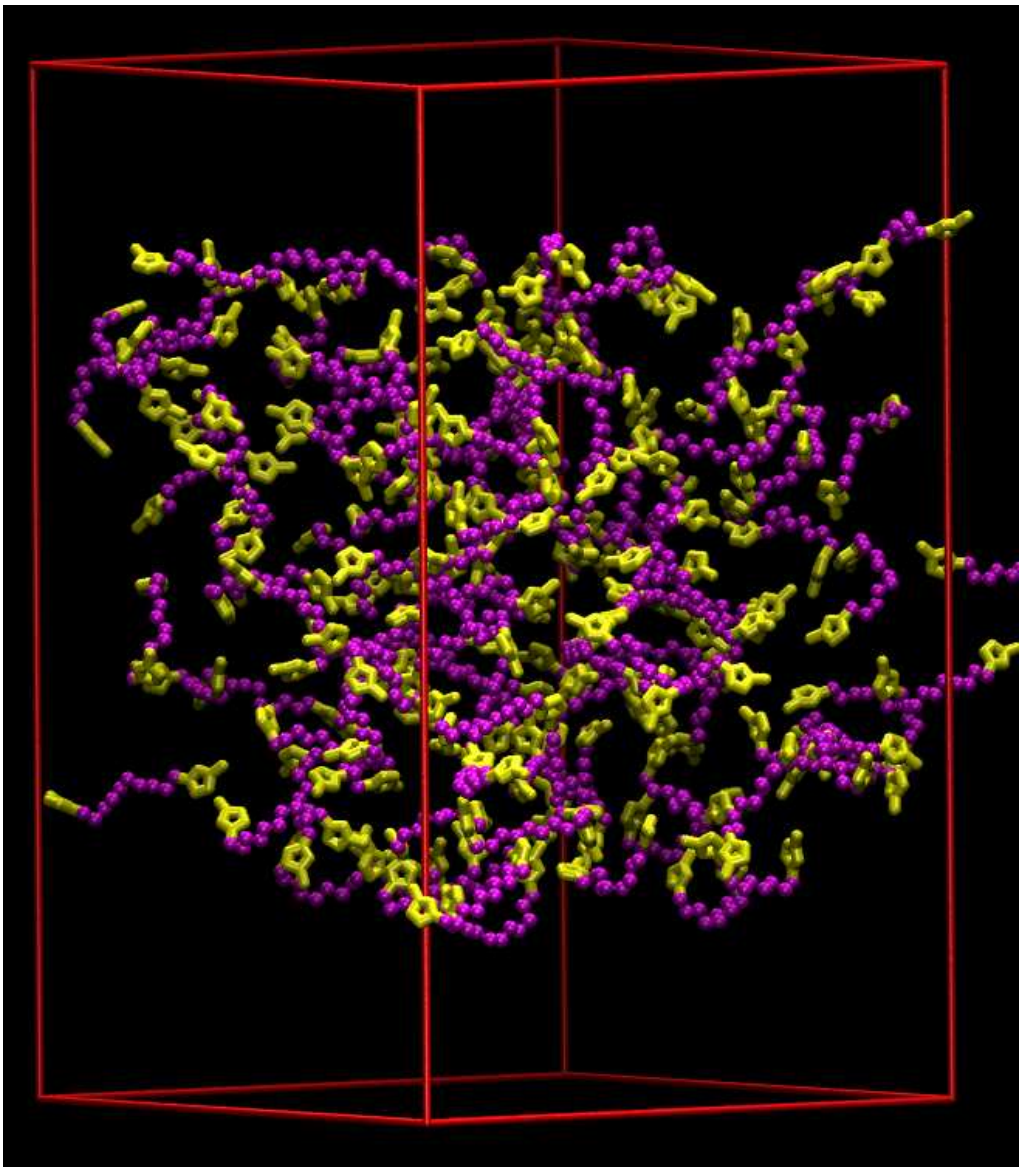

Figure S17: Snapshot of the liquid–vapor interface of aqueous solution of $[C_{10}(MIm)_2][2Br]$ after 25 ns simulations. Head groups are shown in yellow and the tail groups are shown in magenta. Anions, water and hydrogen atoms on the cation are not shown for the ease of visualization.

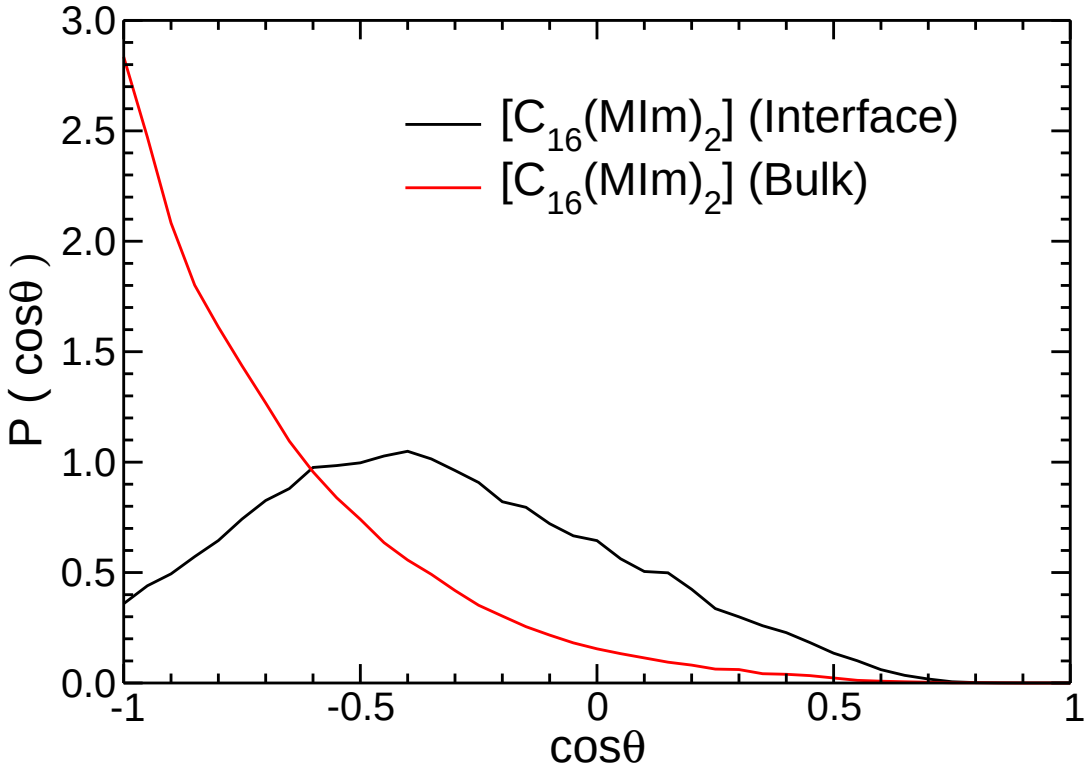

Figure S18: Distribution of angles between the two vectors joining the central carbon atom of the spacer with the imidazolium nitrogen atoms connected to the spacer in the aqueous solution of $[C_{16}(MIm)_2][2Br]$.

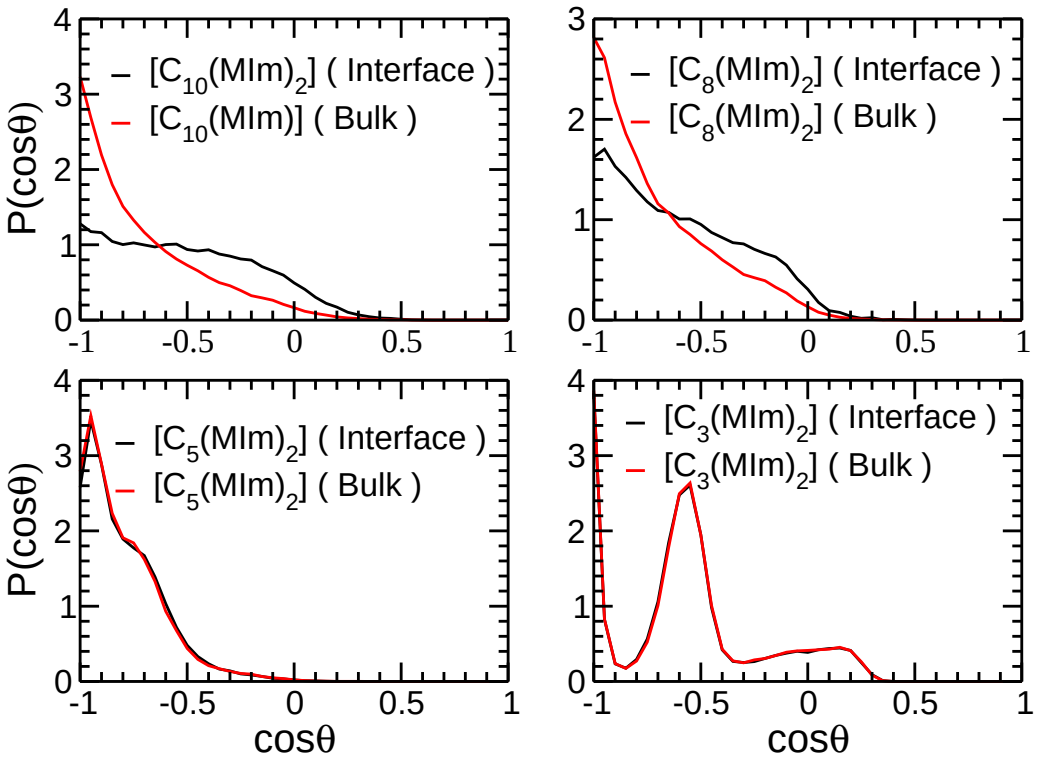

Figure S19: Distribution of angles between the two vectors joining the central carbon atom of the spacer with the imidazolium nitrogen atoms connected to the spacer in the aqueous solution of DILs.