Electronic Supplementary Information

Molecular dynamics simulation of the structure and dynamics in mixtures of ionic liquids and alcohols

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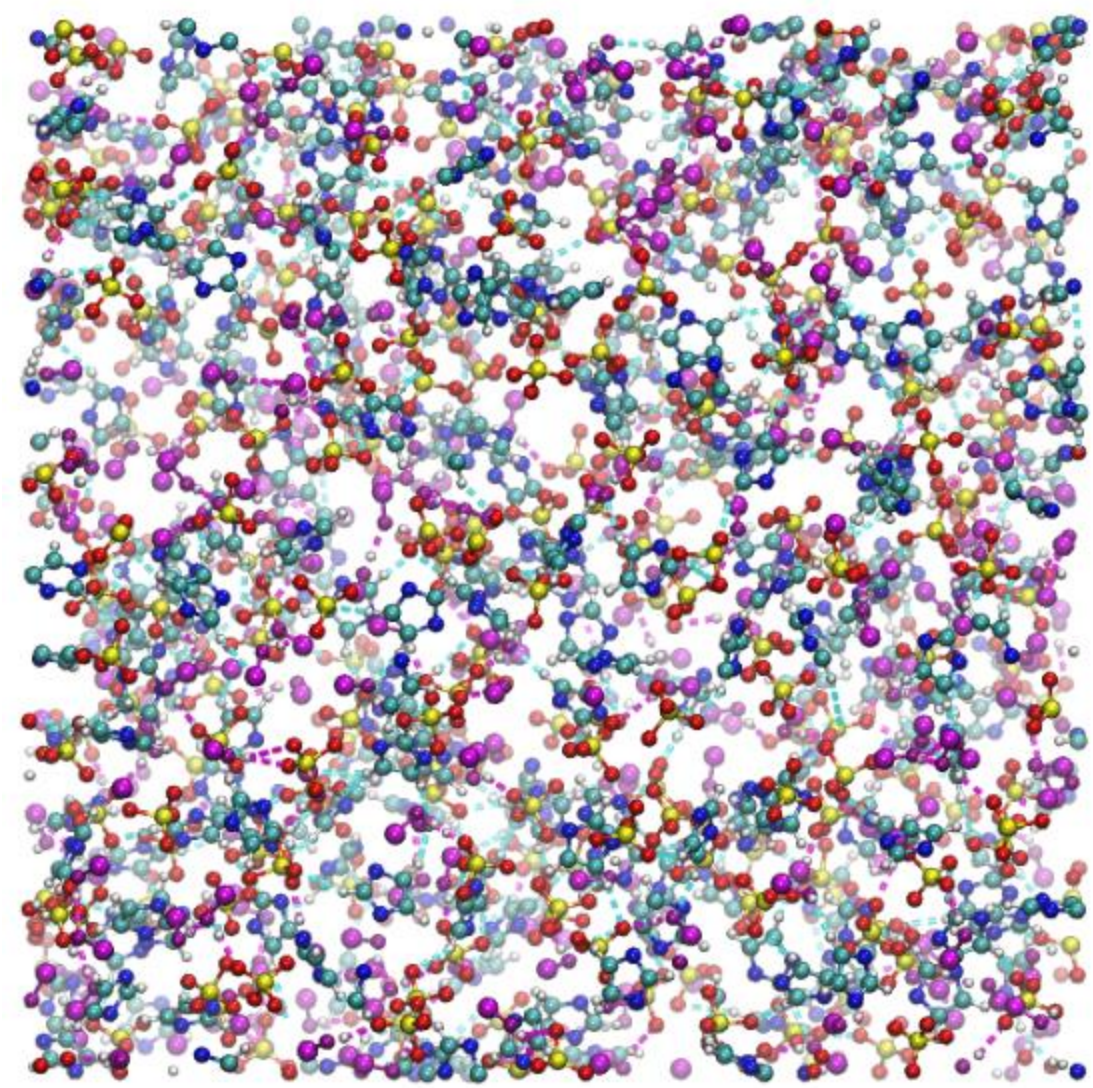

Figure S1. A snapshot of the simulation box for [Bmim][$MeSO_4$]-1-propanol mixture at $x_{1\text{-propanol}}$ = 0.5 is presented. For clarity, the alkyl chain of the cation, the C_2H_5 group from 1-propanol, and the CH_3 group of the anion have been removed. Carbon and nitrogen atoms in the imidazolium ring are represented in cyan and blue, respectively. Oxygen and sulfur in the anion are shown in red and yellow, while the CH_2 group and oxygen of 1-propanol are depicted in purple and magenta, respectively. Hydrogen atoms are indicated in white. The hydrogen bond is highlighted with a cyan or purple dotted line.

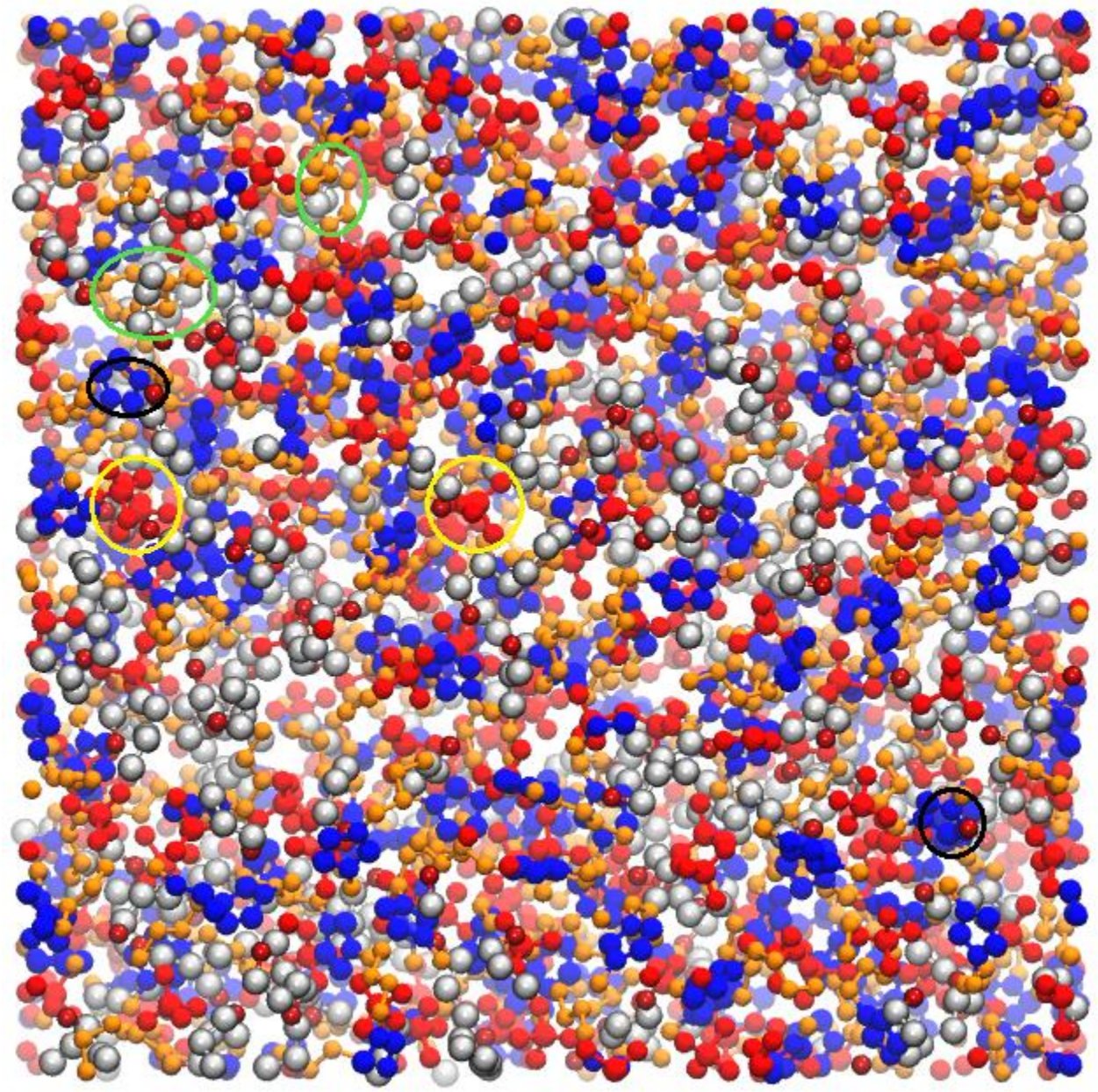

Figure S2. A snapshot of the simulation box for [Bmim][$MeSO_4$]-1-propanol mixture at $x_{1\text{-Propanol}}$ = 0.5 is presented. For clarity, the hydrogen of the cation, propanol and the CH_3 group of the anion have been removed. Carbon and nitrogen atoms in the imidazolium ring are represented in blue, the alkyl group of cations is indicated in orange, the anion is shown in red, while the alkyl group and oxygen of 1-propanol are depicted in white and red, respectively. The neighborhood of the alkyl groups of 1-propanol and cation is illustrated with a light-green circle,

while a yellow circle is used for the 1-propanol oxygen and anion, and a black circle denotes the neighborhoods of the imidazolium ring and the oxygen of 1-propanol.

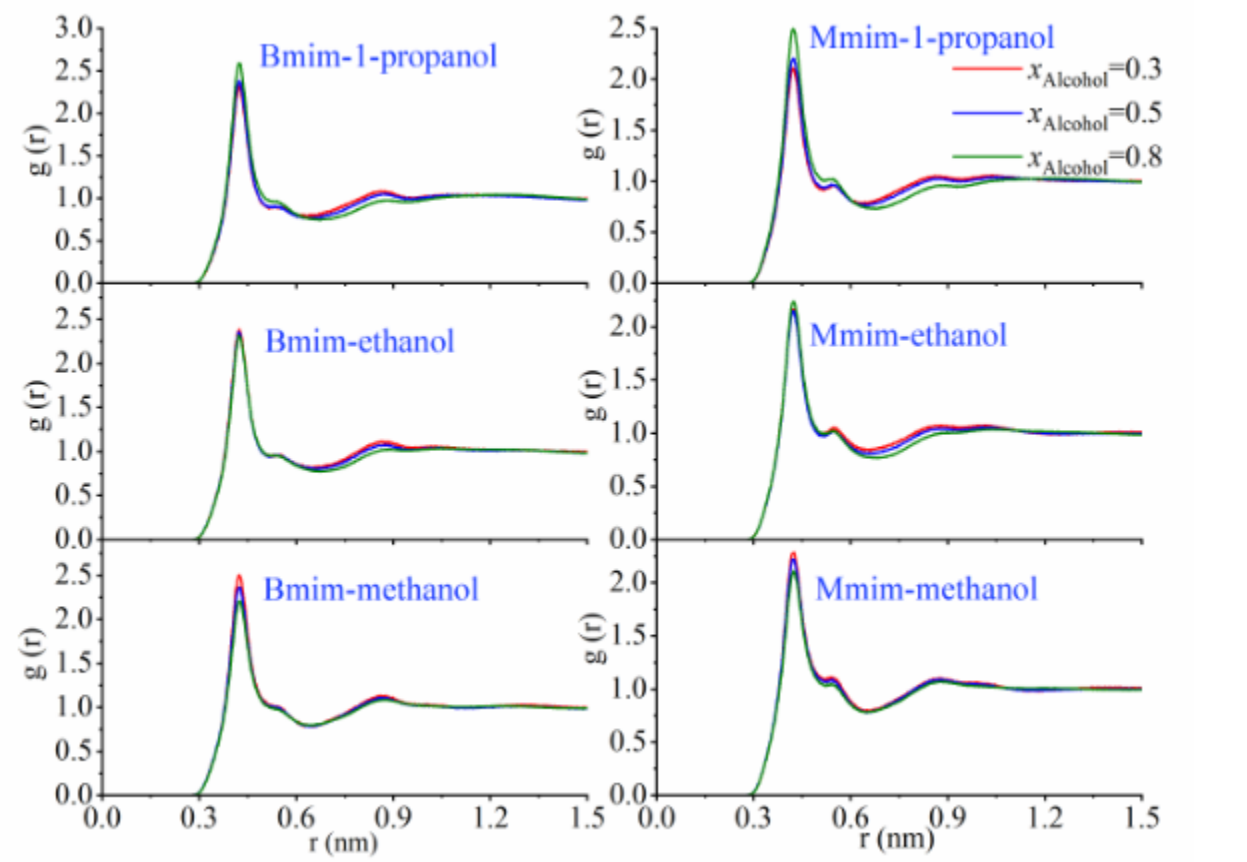

Figure S3. Center-of-mass RDFs between alcohol OH group-imidazolium ring neighbors in [Mmim][$MeSO_4$]-alcohol and [Bmim][$MeSO_4$]-alcohol mixtures at 300 K and 101.3 kPa.

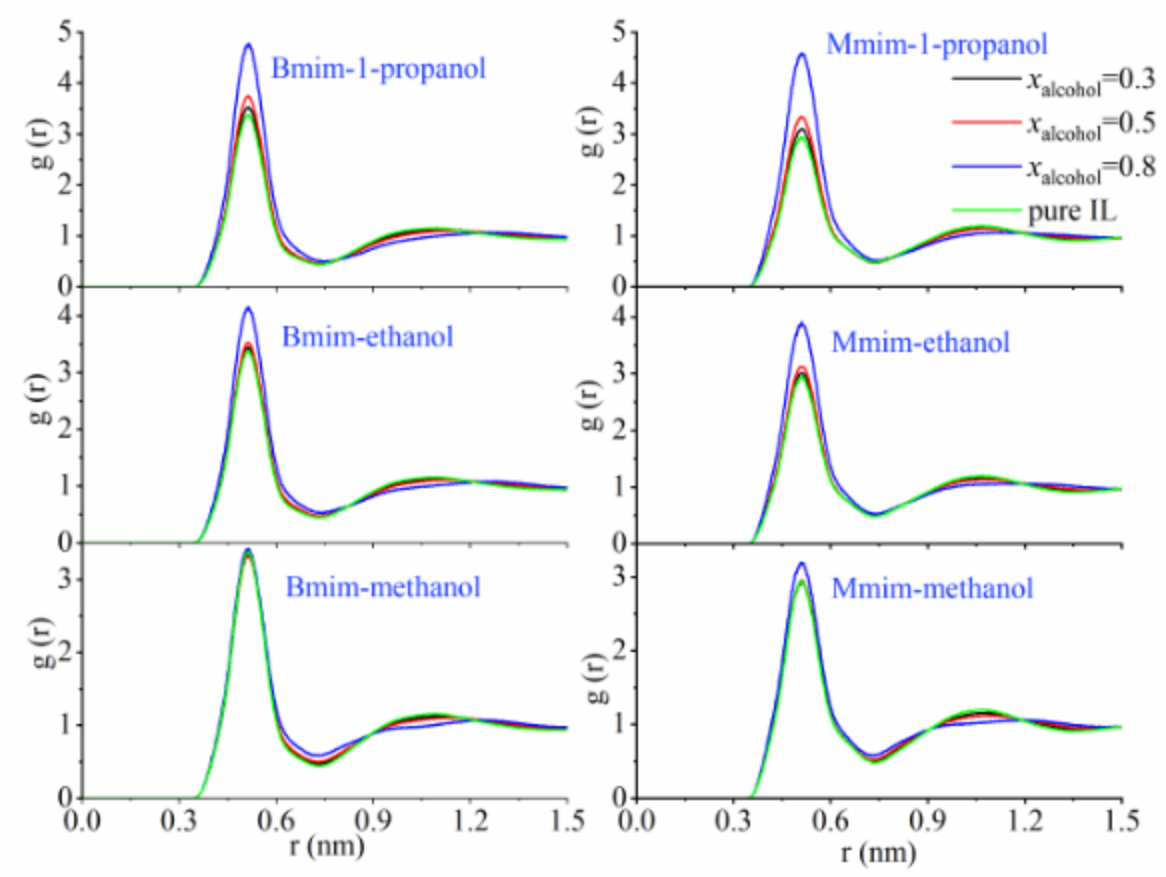

Figure S4. Center-of-mass RDFs between imidazolium ring-anion neighbors in [Mmim][$MeSO_4$]-alcohol and [Bmim][$MeSO_4$]-alcohol mixtures at 300 K and 101.3 kPa.

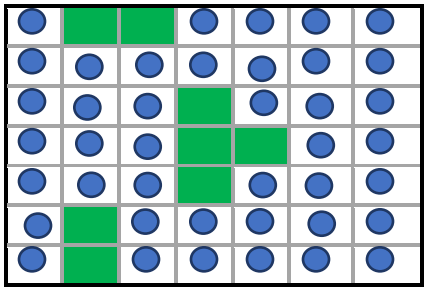

Figure S5. Schematic representation of the grid (grey lines) on a simulation box, used to calculate the free volume. The blue points are the particles existing in the simulation box. The volume of green (unoccupied) cells represent the free volumes.

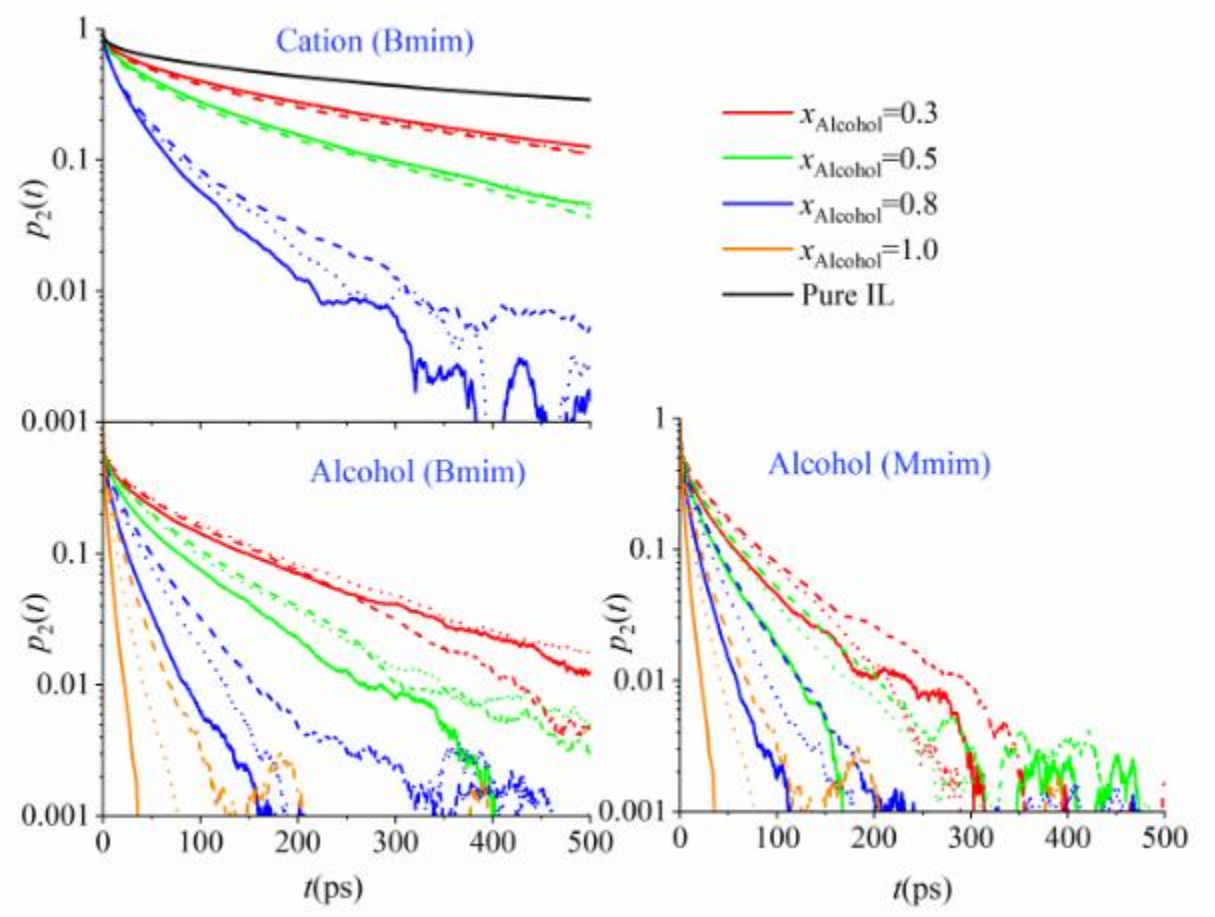

Figure S6. The rotational correlation function of the unit vector aligned with the plane of CH_3OH in methanol, CH_2OH in ethanol, CH_2OH in 1-propanol in [Mmim][$MeSO_4$]-alcohol and [Bmim][$MeSO_4$]- alcohol mixtures, and the alkyl chain of the $[Bmim]^+$ cation in [Bmim][$MeSO_4$]- alcohol mixtures at 300 K and 101.3 kPa. Solid lines, dotted lines, and dashed lines correspond to the IL-methanol, IL-ethanol, and IL-1-propanol mixtures, respectively.

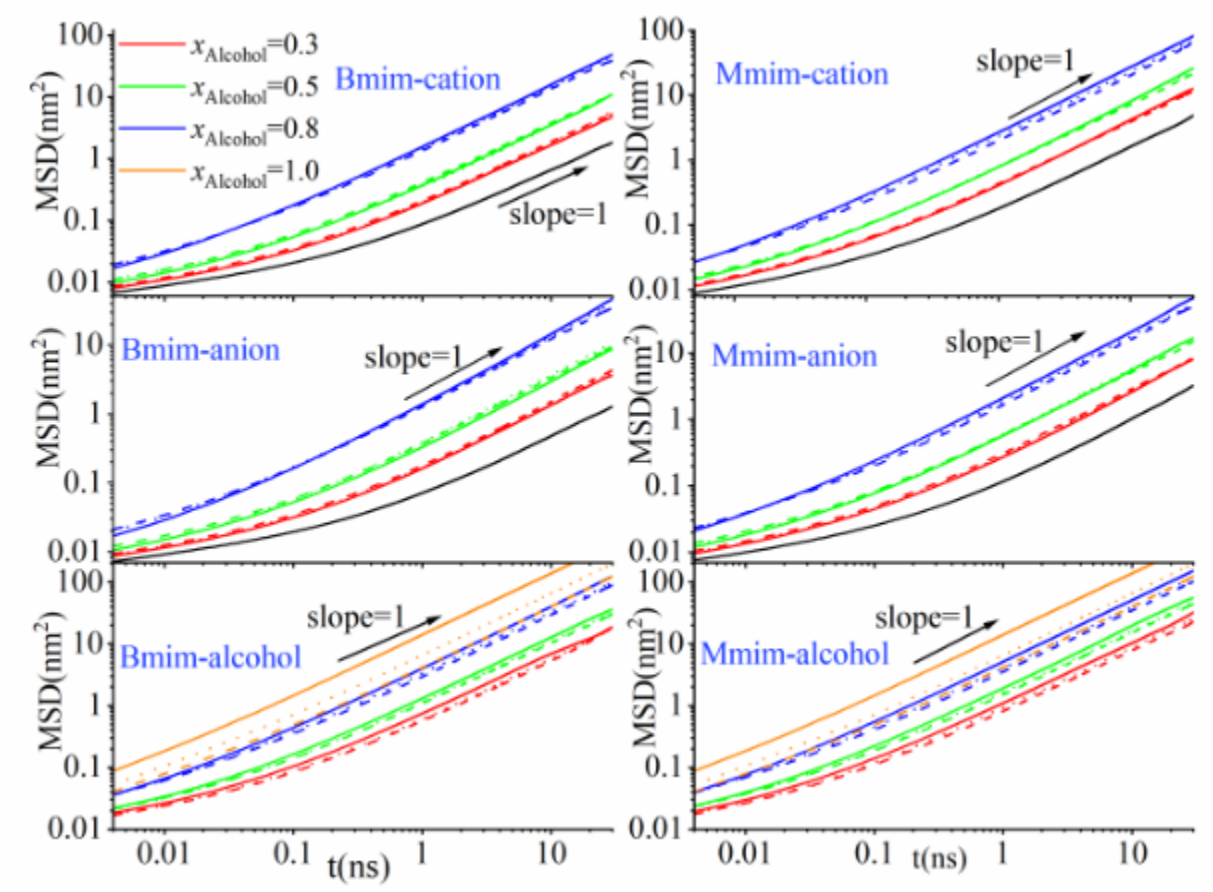

Figure S7. Center-of-mass MSD curves of the cation, anion, and alcohol molecules in [Mmim][$MeSO_4$]-alcohol and [Bmim][$MeSO_4$]-alcohol mixtures at 300 K and 101.3 kPa. Solid lines, dotted lines, and dashed lines correspond to the IL-methanol, IL-ethanol, and IL-1-propanol mixtures, respectively.