Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Investigating the Properties of Fatty Acid-based Ionic Liquids: Advancement in AMOEBA Force Field

Supplimentary Information

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Fragments Used for Parameterization

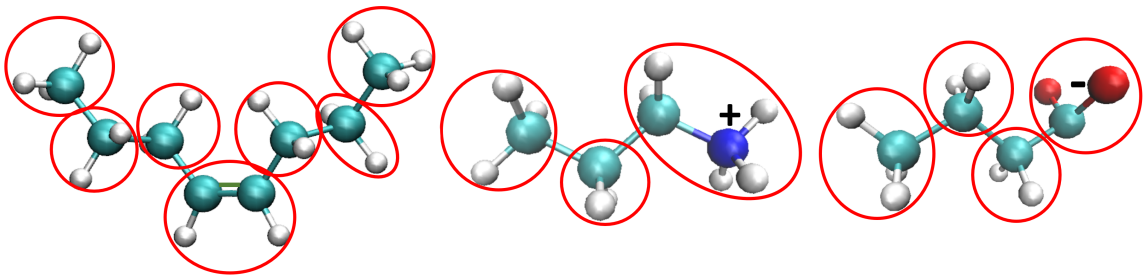

Figure S1: Fragments that are parameterized for $[C_4NH_3]^+[OLE]^-$ ion pair. Distinct polarization groups in parameterization of anion and cation in $[C_4NH_3]^+[OLE]^-$ are $-COO^-$, $-CH_2-$, $-CH_3-$, $-HC{=}CH-$ and $-CH_2\text{-}NH_3^+$ which are defined in red circles.

Compare the Decomposed Energy Calculated by QM and MM for $[EMIM]^+[PALM]^-$

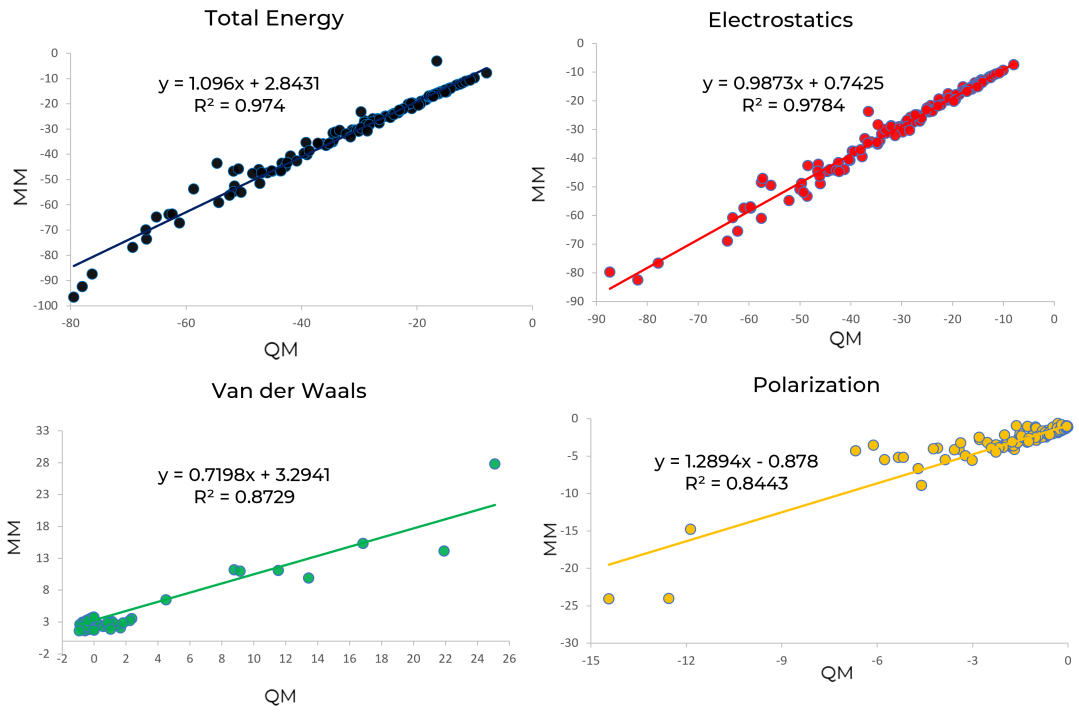

Figure S2: Comparison of intermolecular interaction energies for the $[EMIM]^+[PALM]^-$ ionic pair with randomly varied distances between the anion and cation, using SAPT (QM) and the ANALYZE program in TINKER with the newly developed parameters (MM).

Diffusion Log-Log MSD vs Time Plots

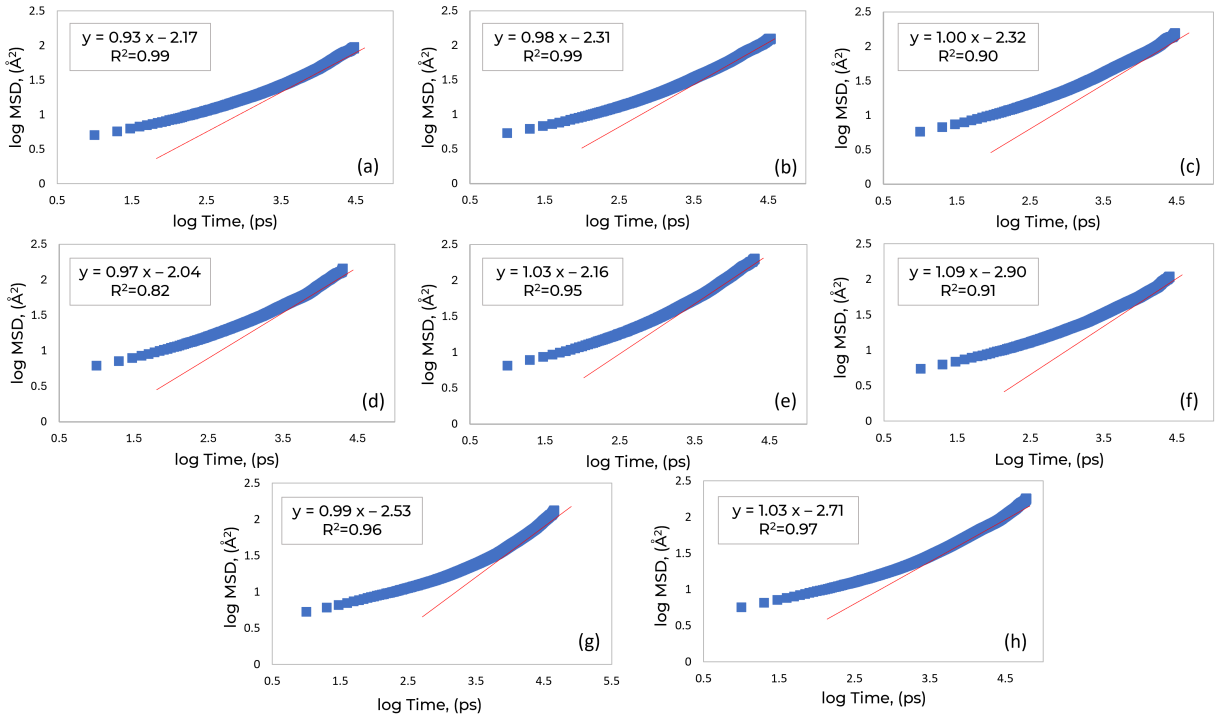

Figure S3: Log MSD vs log time for IL's at different temperatures were ploted. Plots (a), (b), (c), (d), and (e) correspond to $[C_4NH_3]^+[OLE]^-$ at 288.15, 293.15, 298.15, 303.15 and 308.15 K respectively. Plots (f), (g), and (h) correspond to $[NH_4]^+[PALM]^-$ at 298 K and $[EMIM]^+[PALM]^-$ at 315, and 320 K, respectively.

Density and Diffusion Coefficient Calculation Range

Table S1: Total simulation times and trajectory ranges used for determining the averaged density and diffusion coefficients.

Ionic liquid	Temperature (K)	Total Simulation Time (ns)	Trajectory Range (ns)	
			Density (ρ)	Diffusion Coefficient ($D\pm$)
$[C_4NH_3]^+[OLE]^-$	288.15	30	25-30	27-29
	293.15	34	30-34	30-32
	298.15	30	20-30	26-30
	303.15	20	10-20	18-20
	308.15	20	10-20	17.8-20
$[NH_4]^+[PALM]^-$	298	25	20-25	19-25
$[EMIM]^+[PALM]^-$	315	45	35-45	39-44
	320	60	50-60	55-58.5

The Structure Factor Plots

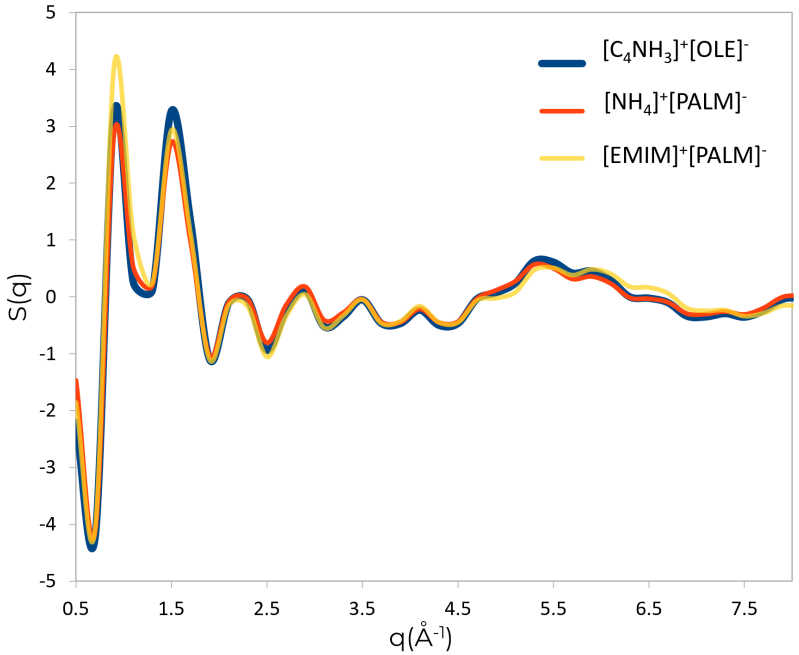

Figure S4: Calculated total structure factor ($S(q)$) for $[C_4NH_3]^+[OLE]^-$ at 298.15 K, $[NH_4]^+[PALM]^-$ at 298 K and $[EMIM]^+[PALM]^-$ at 315 K.