Supporting material

Efficient separation of oil-phenol mixtures and removal of neutral oil entrainment by an in-situ deep eutectic method

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A1 Molecular dynamics simulation details

The GROMACS 2019.1 software package was used to perform MD simulations to determine the molecular-level separation mechanism of DES from MNU. The molecules were randomly distributed in the corresponding area of the simulated box. The particle mesh ewald (PME) method was used to accurately calculate the long-distance electrostatic interaction with a cutoff distance of 12 Å. For the study of liquid properties, periodic boundary conditions (PBC) were used to simulate a small number of particles, and to study macroscopic properties through time averaging. In order to accurately calculate and collect simulation data, the equilibrium phase was calculated using Berendsen thermostat and Berendsen barostat at 25 ℃ and 1 bar, and V-rescale thermostat and Parrinello-Rahman barostat were used to calculate the generated phase. First, the energy of the system was minimized by the steepest descent method, and the minimum system was balanced by the NVT ensemble for 1 ns with a temperature gradient from 0 ℃ to 25 ℃. Then the equilibrium simulation was performed at the isothermal-isobaric ensemble (NPT). Finally, without other constraints, a 50 ns MD simulation was performed in a system with a time step of 2 fs, and the trajectory was analyzed to obtain radial distribution functions (RDFs). The trajectory data was saved every 10 ps, and the trajectory was analyzed and visualized by using VMD software.

Table S1

Compounds and compositions of 180-200 ℃ coal liquefaction oil.

No.	Molecular formula	Compound	Content/%
1	C_9H_{12}	4-Ethyltoluene	0.78
2	$C_{10}H_{18}$	Trans-decalin	11.78
3	$C_{10}H_{18}$	Cis-decaline	4.69
4	$C_{10}H_{14}$	1-Ethyl-2-methyl benzene	1.14
5	C_7H_8O	*o*-Cresol	8.11
6	C_7H_8O	*m*-Cresol	22.55
7	C_7H_8O	*p*-Cresol	22.55
8	$C_{11}H_{24}$	Undecane	7.03
9	C_9H_{12}	3-ethyltoluene	5.00
10	C_9H_{10}	Vinyltoluene	5.35
11	$C_{10}H_{12}$	Tetraline	8.32
12	$C_{12}H_{26}$	Dodecane	2.68

Table S2

Experimental Reagents Information.

Components	Abbreviation	CAS Reg. No.	Purity	Suppliers
m-Cresol	MCR	108-39-4	99%	Macklin Biotechnology Co., Ltd., Shanghai, China
Tetrahydronaphthalene	THN	119-64-2	98.5%	Macklin Biotechnology Co., Ltd., Shanghai, China
Undecane	UND	1120-21-4	99.5%	Macklin Biotechnology Co., Ltd., Shanghai, China
1-Ethyl-3-methylimidazolium chloride	LC	65039-09-0	98%	Macklin Biotechnology Co., Ltd., Shanghai, China
Choline chloride	ChCl	67-48-1	99%	Aladdin Biotechnology Co., Ltd., Shanghai, China
Glycerol	Gly	56-81-5	99%	Macklin Biotechnology Co., Ltd., Shanghai, China

Table S3

Partial charges of different atoms in the molecule species.

Atom Type	Partial Charge	Atom Type	Partial Charge	Atom Type	Partial Charge	Atom Type	Partial Charge
Emim		THN		UND		Ch	
N1	0.11	C1	−0.07	C1	−0.25	C1	−0.08
C1	−0.13	C2	0.05	C2	0.21	N1	0.04
C2	−0.18	C3	0.05	C3	0.01	C2	0.26
C3	−0.04	C4	−0.08	C4	0.03	C3	−0.33
N2	0.26	C5	0.07	C5	0.10	C4	−0.41
C4	−0.18	C6	−0.20	C6	0.04	C5	−0.33
C5	−0.08	C7	−0.13	C7	0.10	O1	−0.61
C6	−0.35	C8	−0.13	C8	0.03	H1	0.14
H1	0.22	C9	−0.20	C9	0.01	H2	0.14
H2	0.24	C10	0.07	C10	0.21	H3	0.01
H3	0.10	H1	0.03	C11	−0.25	H4	0.01
H4	0.10	H2	0.03	H1	0.05	H5	0.18
H5	0.23	H3	−0.01	H2	0.05	H6	0.18
H6	0.06	H4	−0.01	H3	0.05	H7	0.18
H7	0.06	H5	−0.01	H4	−0.04	H8	0.20
H8	0.06	H6	−0.01	H5	−0.04	H9	0.20
H9	0.17	H7	0.03	H6	−0.02	H10	0.20
H10	0.17	H8	0.03	H7	−0.02	H11	0.18
H11	0.17	H9	0.12	H8	−0.03	H12	0.18
MCR		H10	0.12	H9	−0.03	H13	H13
C1	−0.37	H11	0.12	H10	−0.04	H14	0.44
C2	0.34	H12	0.12	H11	−0.04	Gly	
C3	−0.43			H12	−0.03	C1	0.16
C4	0.47			H13	−0.03	C2	0.10
C5	−0.40			H14	−0.04	C3	0.13
C6	−0.01			H15	−0.04	O1	−0.61
H1	0.16			H16	−0.03	O2	−0.58
H2	0.20			H17	−0.03	O3	−0.58
H3	0.16			H18	−0.02	H1	0.01
H4	0.12			H19	−0.02	H2	0.01

C7	−0.33	H20	−0.04	H3	0.09
H5	0.09	H21	−0.04	H4	0.05
H6	0.09	H22	0.05	H5	0.05
H7	0.09	H23	0.05	H6	0.41
O1	−0.58	H24	0.05	H7	0.39
H8	0.40			H8	0.39

Table S4

Lennard-Jones parameters used for $[Emim]^+$, $[Ch]^+$, $[Cl]^-$, Gly, MCR, THN and UND.

Atom Type	ε (kcal/mol)	σ	Atom Type	ε (kcal/mol)	σ
	$[Emim]^+$			Gly	
na	0.3250	0.7113	c3	0.3400	0.4577
cc	0.3400	0.3598	oh	0.3066	0.8803
c3	0.3400	0.4577	h1	0.2471	0.0657
cd	0.3400	0.3598	ho	0.0000	0.0000
h5	0.2421	0.0628		MCR	
h4	0.2511	0.0628	ca	0.3400	0.3598
h1	0.2471	0.0657	ha	0.2600	0.0628
hc	0.2650	0.0657	c3	0.3400	0.4577
	$[Ch]^+$		hc	0.2650	hc
c3	0.3400	0.4577	oh	0.3066	0.8803
n4	0.3250	0.7113	ho	0.0000	0.0000
oh	0.3066	0.8803		THN	
hx	0.1960	0.0657	c3	0.3400	0.4577
h1	0.2471	0.0657	ca	0.3400	0.3598
	UND		ha	0.2600	hc
c3	0.3400	0.4577	ha	0.2600	0.0628
hc	0.2650	0.0657		$[Cl]^-$	
			cl	0.3471	1.1088

Table S5

Bonded parameters used for $[Emim]^+$, $[Ch]^+$, Gly, MCR, THN and UND.

Bonds-Type	*r*	*k*
	$[Emim]^+$	
N1 - C1	0.1380	356310
N1 - C2	0.1380	356310
N1 - C3	0.1463	274220
C1 - N2	0.1380	356310
C1 - H1	0.1082	294300
C2 - C4	0.1373	419150
C2 - H2	0.1082	294550
C3 - C5	0.1538	251790
C3 - H3	0.1097	276650
C3 - H4	0.1097	276650
N2 - C4	0.1380	356310
N2 - C6	0.1463	274220
C4 - H5	0.1082	294550
C5 - H6	0.1097	276650
C5 - H7	0.1097	276650
C5 - H8	0.1097	276650
C6 - H9	0.1097	276650
C6 - H10	0.1097	276650
C6 - H11	0.1097	276650
	$[Ch]^+$	
C1 - N1	0.1511	237070
C1 - C2	0.1538	251790
C1 - H1	0.1091	283420
C1 - H2	0.1091	283420
N1 - C3	0.1511	237070
N1 - C4	0.1511	237070
N1 - C5	0.1511	237070
C2 - O1	0.1423	265010
C2 - H3	0.1097	276650
C2 - H4	0.1097	276650
C3 - H5	0.1091	283420
C3 - H6	0.1091	283420
C3 - H7	0.1091	283420
C4 - H8	0.1091	283420
C4 - H9	0.1091	283420
C4 - H10	0.1091	283420
C5 - H11	0.1091	283420
C5 - H12	0.1091	283420

C5 - H13	0.1091	283420
O1 - H14	0.0973	310790
	Gly	
C1 - C2	0.1538	251790
C1 - O1	0.1423	265010
C1 - H1	0.1097	276650
C1 - H2	0.1097	276650
C2 - C3	0.1538	251790
C2 - O2	0.1423	265010
C2 - H3	0.1097	276650
C3 - O3	0.1423	265010
C3 - H4	0.1097	276650
C3 - H5	0.1097	276650
O1 - H6	0.0973	310790
O2 - H7	0.0973	310790
O3 - H8	0.0973	310790
	MCR	
C1 - C2	0.1398	385850
C1 - C6	0.1398	385850
C1 - H1	0.1086	289370
C2 - C3	0.1398	385850
C2 - C7	0.1516	268610
C3 - C4	0.1398	385850
C3 - H2	0.1086	289370
C4 - C5	0.1398	385850
C4 - O1	0.1364	321330
C5 - C6	0.1398	385850
C5 - H3	0.1086	289370
C6 - H4	0.1086	289370
C7 - H5	0.1097	276650
C7 - H6	0.1097	276650
C7 - H7	0.1097	276650
O1 - H8	0.0973	310790
	THN	
C1 - C2	0.1538	251790
C1 - C10	0.1516	268610
C1 - H1	0.1097	276650
C1 - H2	0.1097	276650
C2 - C3	0.1538	251790
C2 - H3	0.1097	276650
C2 - H4	0.1097	276650
C3 - C4	0.1538	251790
C3 - H5	0.1097	276650
C3 - H6	0.1097	276650

C4 - C5	0.1516	268610
C4 - H7	0.1097	276650
C4 - H8	0.1097	276650
C5 - C6	0.1398	385850
C5 - C10	0.1398	385850
C6 - C7	0.1398	385850
C6 - H9	0.1086	289370
C7 - C8	0.1398	385850
C7 - H10	0.1086	289370
C8 - C9	0.1398	385850
C8 - H11	0.1086	289370
C9 - C10	0.1398	385850
C9 - H12	0.1086	289370
	UND	
C1 - C2	0.1538	251790
C1 - H1	0.1097	276650
C1 - H2	0.1097	276650
C1 - H3	0.1097	276650
C2 - C3	0.1538	251790
C2 - H4	0.1097	276650
C2 - H5	0.1097	276650
C3 - C4	0.1538	251790
C3 - H6	0.1097	276650
C3 - H7	0.1097	276650
C4 - C5	0.1538	251790
C4 - H8	0.1097	276650
C4 - H9	0.1097	276650
C5 - C6	0.1538	251790
C5 - H10	0.1097	276650
C5 - H11	0.1097	276650
C6 - C7	0.1538	251790
C6 - H12	0.1097	276650
C6 - H13	0.1097	276650
C7 - C8	0.1538	251790
C7 - H14	0.1097	276650
C7 - H15	0.1097	276650
C8 - C9	0.1538	251790
C8 - H16	0.1097	276650
C8 - H17	0.1097	276650
C9 - C10	0.1538	251790
C9 - H18	0.1097	276650
C9 - H19	0.1097	276650
C10 - C11	0.1538	251790
C10 - H20	0.1097	276650

C10 - H21	0.1097	276650
C11 - H22	0.1097	276650
C11 - H23	0.1097	276650
C11 - H24	0.1097	276650

Table S6

Experimental initial feed composition and considered number of molecules in MD simulations.

DESs type	Number of molecules						
	Ch^+	Gly	$Emim^+$	Cl^-	MCR	THN	UND
EmimCl:MCR			200	200	280	200	100
ChCl:MCR	200			200	480	200	100
ChCl:Gly	200	200		200	200	200	100

Table S7

LLE data of MCR(1) - THN(2) - UND(3) - Emimcl(4).

No.	Raffinate phase				Extract phase			
	x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
1	0.0002	0.2113	0.7884	0	0.4529	0.0429	0.0511	0.4530
2	0.0005	0.3622	0.6373	0	0.4445	0.0735	0.0390	0.4430
3	0.0006	0.4803	0.5190	0	0.4302	0.0977	0.0417	0.4304
4	0.0010	0.5597	0.4393	0	0.4254	0.1138	0.0349	0.4258
5	0.0007	0.6227	0.3766	0	0.4165	0.1332	0.0352	0.4150
6	0.0008	0.6677	0.3315	0	0.4125	0.1420	0.0326	0.4129
7	0.0008	0.7042	0.2951	0	0.4043	0.1593	0.0317	0.4047
8	0.0008	0.7354	0.2638	0	0.4000	0.1686	0.0308	0.4006
9	0.0009	0.7603	0.2388	0	0.4029	0.1674	0.0262	0.4035

Table S8

Binary interaction parameters Δb_{ij}, Δb_{ji} for NRTL model.

i-j	Δb_{ij} /(kJ·mol^{-1})	Δb_{ji} /(kJ·mol^{-1})
MCR(1) - THN(2) - UND(3) - EmimCl(4)		
1-2	−107.32	852.96
1-3	2151.61	−849.56
1-4	−2462.04	2132.96
2-3	274.41	−113.49
2-4	1050.14	2037.90
3-4	1334.40	1474.17

Table S9

Modified Group Contribution method.

	Model equation	Constants
The method	$T_b = 198.2 + \sum n_i \Delta T_b$	$A = 0.5703$
	$T_c = \frac{T_b}{A + B\sum n_i \Delta T_c - (\sum n_i \Delta T_c)^2}$	$B = 1.0121$
	$P_c = \frac{M}{C + (\sum n_i \Delta P_c)^2}$	$C = 0.2573$
	$V_c = D + \sum n_i \Delta V_c$	$D = 6.75$
Density model for testing	$\rho(\mathrm{g/cm^3}) = (A/B)+(2/7)\cdot\{(A\cdot \mathrm{Ln}B)/B\}^{\frac{T - T_b}{T_c - T_b}}$	$A = a+b\cdot M/V_c$ $B = (c/V_c+d/M)\cdot V_c^{\delta}$ $A = 0.3411$, b=2.0443, c = 0.5386, $d = 0.0393$, $e = 1.0476$
Critical compressibility factor	$Z_c = P_c V_c / RT_c$	$R = 84.31$ (bar cm^3/mol K)
Acentric factor	$\omega = \frac{(T_b - 43)(T_c - 43)}{(T_c - T_b)(0.7T_c - 43)}\mathrm{Log}[\frac{P_c}{P_b}]$ $- \frac{(T_c - 43)}{(T_c - T_b)}\mathrm{Log}[\frac{P_c}{P_b}] + \mathrm{Log}[\frac{P_c}{P_b}] - 1$	$P_b = 1.01325$ bar

In the equations, M is in g/mol, T_b and T_c in K, P_c in bar and V_c in (cm^3/mol).

Table S10

Physical properties of the EmimCl at 298.15 K and atmospheric pressure.

Items	Units	EmimCl
T_c	K	748.6
V_c	mL mol^{-1}	454.5
P_c	bar	34.17
T_b	K	512.3
Z_c		0.2495
ω		0.4165

Table S11

Basis of economics and equipment sizing.

Items	Formulas and values
column vessel	column diameter = Aspen tray sizing column length = N_T trays with 2 ft spacing plus 20% extra length investment cost=$17640D^{1.066}L^{0.802}$, where D and L are in m
Reboilers	heat-transfer coefficient (K_R)=0.568kW/ (K·m^2) differential temperature (ΔT_R) =steam temperature – base temperature $A_R = \frac{Q_R}{K_R \times \Delta T_R}$ capital cost=7296 $(A_R)^{0.65}$
Coolers	heat-transfer coefficient (K_C)=0.852kW/ (K·m^2) differential temperature (ΔT_C) = log-mean temperature difference of inlet and outlet temperature differences $A_C = \frac{Q_C}{K_C \times \Delta T_C}$ capital cost=7296 $(A_C)^{0.65}$
Extraction column	length: N_T trays with 4 ft HETP plus additional 3 ft at the top and 3 ft at the bottom capital cost = $17640(D)^{1.066}$ $(L)^{0.802}$ (D and L are in meters)
Utilities cost	low pressure steam (160 ℃) = \$7.78/GJ medium pressure steam (184 ℃) = \$8.22/GJ high pressure steam (254 ℃) = \$9.88/GJ cooling water = \$0.354/GJ cold water = \$0.443/GJ Electricity = \$0.094/kW·h
Vacuum system	W'[1b/h] = $5+(0.0298+0.03088\ln P-0.0005733(\ln P)^2)\ V^{0.66}$ Vacuum system cost [\$] = $1690\times1.8\times(W'/P)^{0.41}$ P [$torr$] is the vacuum pressure and V[ft^3] is the volume of the vessel
TAC = (investment cost/ plant life time) + operating cost plant life time = 3 years	

Table S12

Data of FIGURE 2(A).

HBA	*D*	*S*	*PI*
2-mim	1.06	6.91	7.32
TEPC	14.44	227.37	3283.22
TEAC	21.25	196.05	4166.06
TPAC	8.85	193.90	1716.02
emimCl	8.11	166.11	1347.15
TMPC	8.59	155.42	1335.06
ETPPB	8.20	74.69	612.46
MTPPB	19.65	123.11	2419.11
TEMAC	9.77	118.20	1154.81
Lcar	8.14	115.95	943.83
TMAB	7.22	109.51	790.66
TEPB	10.97	102.86	1128.37
TBAC	8.50	101.68	864.28
ChBr	10.11	96.05	971.07
ChCl	9.22	91.68	845.29
TPAB	6.59	91.00	599.69
emimbr	7.48	87.86	657.19
BTMAC	6.51	68.68	447.11
TMAC	4.73	65.92	311.80
bmimcl	6.43	46.59	299.57
TEAB	5.24	42.50	222.70
IM	0.96	16.34	15.69
TBPC	2.50	5.07	12.68
bmimbr	1.70	2.98	5.07
TMAHC	1.23	2.92	3.59
EAHC	1.01	2.88	2.91

Table S13

The lowest molar ratio of liquid DES synthesized by various HBA and MCR at 25 °C.

HBA type	L-car	EmimCl	TEMAC	TEAC	TPAC	ChCl	TEPC
HBA:MCR	1:1.8	1:0.4	1:2.1	1:1.2	1:1.1	1:1.4	1:1.5

Table S14

The interaction energy between molecules in different systems.

Molecular pair	Van der Waals interaction (E_{vdW})	Electrostatic interactions (E_{elec})	Total nonbonded interactions (E_{total})
EmimCl:MCR(1:0.4), (A:$Emim^+$, B:Cl^-, C:MCR, D:THN, E:UND)			
AB	−881.75	0.18	−881.57
AC	1.26	−13.93	−12.68
BC	−45.96	4.05	−41.91
AD	1.14	−1.45	−0.31
BD	−1.44	−0.17	−1.61
AE	−0.28	−0.27	−0.55
BE	0.28	−0.04	0.24
CD	−0.42	−7.54	−7.96
CE	−0.01	−4.46	−4.47
AB-C	−44.70	−9.88	−54.59
(AB+1.4×C)-DE	−0.90	−18.73	−19.63
ChCl:MCR(1:1.4), (A:Ch^+, B:Cl^-, C:MCR, D:THN, E:UND)			
AB	−781.21	5.93	−775.29
AC	5.20	−12.42	−7.22
BC	−46.90	4.07	−42.83
AD	0.55	−0.70	−0.14
BD	−0.82	−0.10	−0.91
AE	−0.31	−0.37	−0.68
BE	0.31	−0.06	0.25
CD	−0.62	−7.65	−8.27
CE	−0.01	−4.84	−4.84
AB-C	−41.70	−8.35	−50.05
(AB+2.4×C)-DE	−1.77	−31.18	−32.96
ChCl:Gly(1:1), (A:Ch^+, B:Cl^-, C:MCR, D:THN, E:UND, F:Gly)			
AB	−831.25	4.60	−826.65
AF	−3.57	−15.66	−19.23
BF	−82.25	9.02	−73.23
AC	1.99	−5.35	−3.36
BC	−25.87	2.06	−23.81
FC	0.52	−4.57	−4.05

AD	0.77	−1.41	−0.63
BD	−1.31	−0.21	−1.51
FD	−0.10	−2.03	−2.13
AE	−0.38	−0.50	−0.88
BE	0.38	−0.09	0.29
FE	0.00	−1.09	−1.10
CD	−0.68	−9.13	−9.81
CE	−0.01	−5.63	−5.63
ABF-C	−23.36	−7.86	−31.23
ABF-DE	−1.33	−20.07	−21.40

Table S15

Atomic contribution to dispersion energy.

Atom Type	Dispersion energy	Atom Type	Dispersion energy	Atom Type	Dispersion energy	Atom Type	Dispersion energy
$Emim^+$		THN		UND		Ch^+	
N1	−1.85	C1	−1.73	C1	−0.97	C1	−2.07
C1	−2.07	C2	−1.56	C2	−1.29	N1	−1.98
C2	−1.82	C3	−1.56	C3	−1.52	C2	−1.63
C3	−1.53	C4	−1.73	C4	−1.57	C3	−1.81
N2	−1.67	C5	−2.46	C5	−1.59	C4	−1.59
C4	−1.69	C6	−1.91	C6	−1.58	C5	−1.57
C5	−1.26	C7	−1.61	C7	−1.58	O1	−0.89
C6	−1.27	C8	−1.61	C8	−1.57	H1	−0.79
H1	−0.78	C9	−1.91	C9	−1.52	H2	−0.95
H2	−0.61	C10	−2.46	C10	−1.29	H3	−0.79
H3	−0.65	H1	−0.65	C11	−0.97	H4	−0.60
H4	−0.58	H2	−0.70	H1	−0.39	H5	−0.65
H5	−0.54	H3	−0.56	H2	−0.45	H6	−0.85
H6	−0.42	H4	−0.69	H3	−0.45	H7	−0.73
H7	−0.66	H5	−0.69	H4	−0.59	H8	−0.61
H8	−0.55	H6	−0.56	H5	−0.59	H9	−0.63
H9	−0.48	H7	−0.65	H6	−0.68	H10	−0.73
H10	−0.61	H8	−0.70	H7	−0.68	H11	−0.62
H11	−0.48	H9	−0.61	H8	−0.69	H12	−0.61
MCR		H10	−0.50	H9	−0.69	-0.69	H13
C1	−1.77	H11	−0.50	H10	−0.70	H14	−0.59
C2	−1.90	H12	−0.61	H11	−0.70	Gly	
C3	−1.86			H12	−0.70	C1	−1.19
C4	−1.71			H13	−0.70	C2	−1.34
C5	−1.66			H14	−0.70	C3	−1.15
C6	−1.60			H15	−0.70	O1	−0.75
H1	−0.58			H16	−0.69	O2	−0.95
H2	−0.62			H17	−0.69	O3	−0.70
H3	−0.54			H18	−0.68	H1	−0.55
H4	−0.50			H19	−0.68	H2	−0.52
C7	−1.14			H20	−0.59	H3	−0.61
H5	−0.47			H21	−0.59	H4	−0.50
H6	−0.48			H22	−0.39	H5	−0.54
H7	−0.48			H23	−0.45	H6	−0.34
O1	−0.80			H24	−0.45	H7	−0.49
H8	−0.42					H8	−0.43

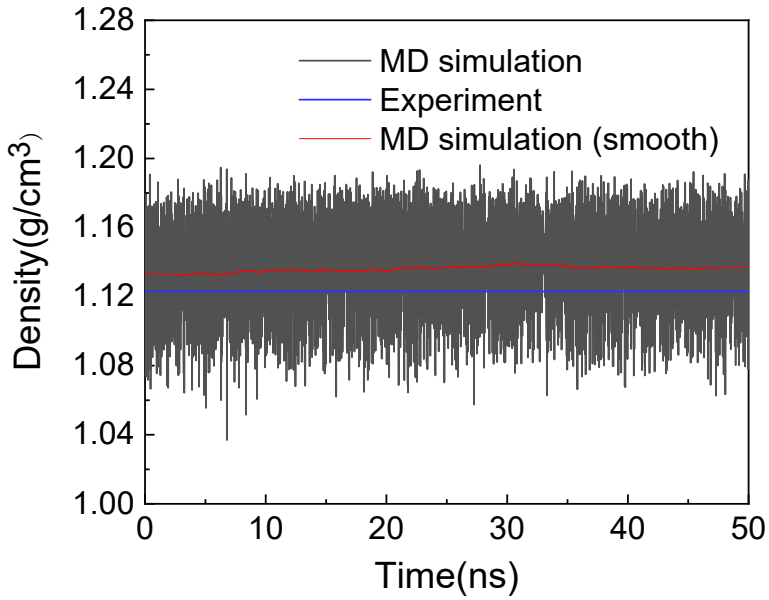

Fig. S1. The experimental and MD simulated density values of EmimCl at 298.15 K (Experiment: 1.123, MD: 1.138).

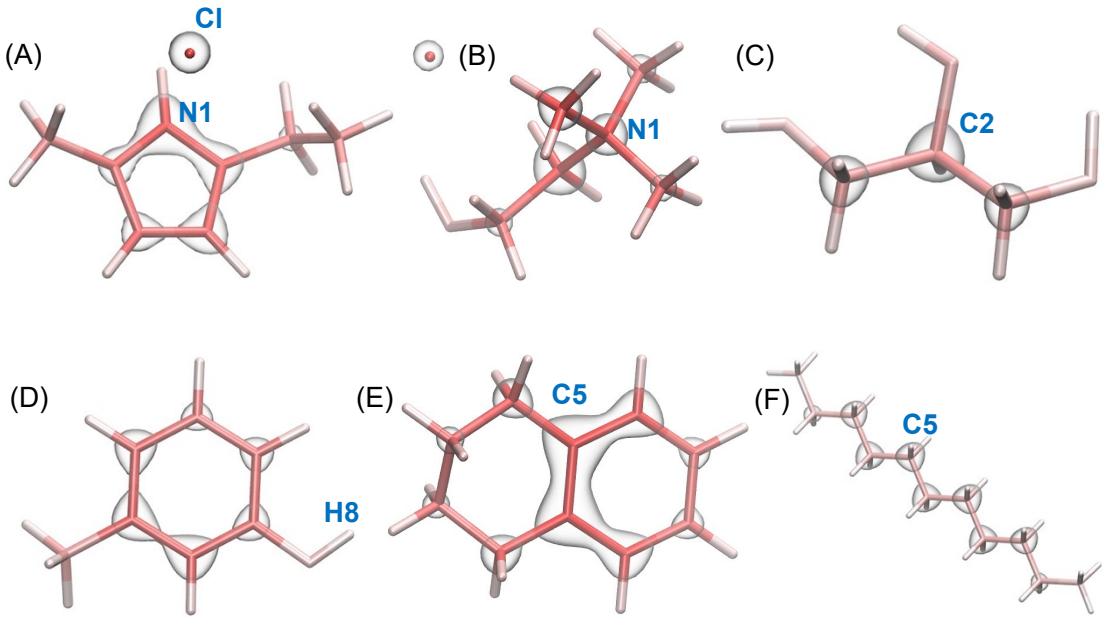

Fig. S2. Dispersion energy density diagram of EmimCl (A), ChCl (B), Gly (C), MCR (D), THN (E), UND (F), and their reference atoms in RDF analysis.