Electronic supplementary information

for

Glucose-Water-Urea Deep Eutectics: How Water Structure and Dynamics Alters in a Crowded Environment

Atanu Baksi, Juriti Rajbangshi and Ranjit Biswas[*]

Department of Chemical, Biological and Macromolecular Sciences, S. N. Bose National Centre for Basic Sciences, JD Block, Sector-III, Salt Lake, Kolkata 700106, INDIA.

[*] Address for correspondence: ranjit@bose.res.in; phone: +91 33 2335 5706; FAX: +91 33 2335 3477
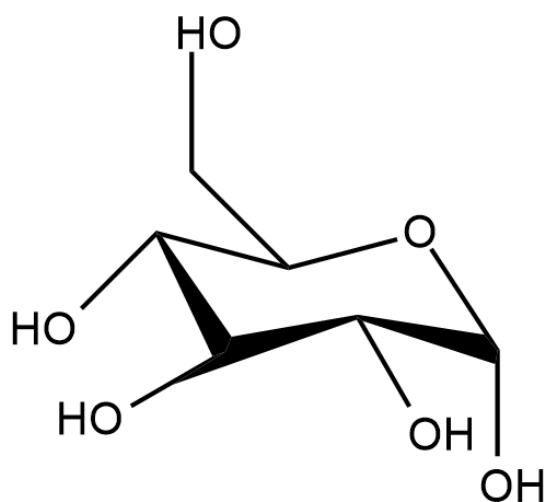
Scheme S1: Schematic representation of chair form of glucose molecule employed in the present simulation study.
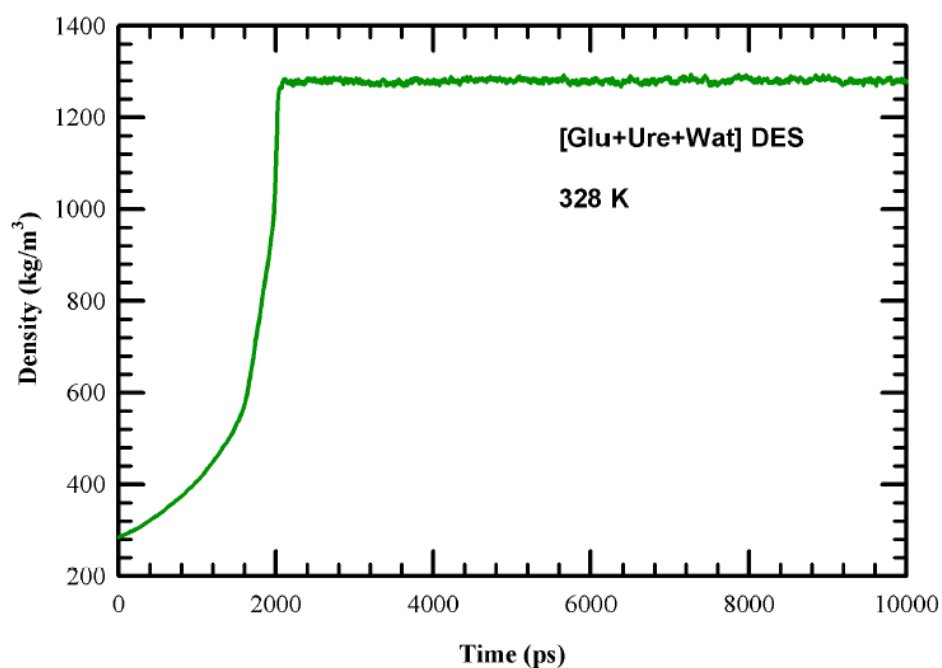

Figure S1: Time evolution of density of the [Glu+Ure+wat] DES during 10 ns NPT simulation run at a temperature 328 K.

Table S1: Atomic charges and non-bonded parameters for glucose molecule.

atom	charge	σ (nm)	ε_i (kJ/mol)
H00	0.4166	0.00	0.00
O01	-0.6744	0.312	0.711
C02	0.1208	0.35	0.276
H03	0.1187	0.25	0.1255
H04	0.1187	0.25	0.1255
C05	0.0342	0.35	0.276
H06	0.118	0.25	0.1255
C07	0.141	0.35	0.276
H08	0.1292	0.25	0.1255
O09	-0.6712	0.312	0.711
H0A	0.4349	0.00	0.00
C0B	0.1285	0.35	0.276
H0C	0.1117	0.25	0.1255
O0D	-0.6833	0.312	0.711
H0E	0.4339	0.00	0.00
C0F	0.0638	0.35	0.276
H0G	0.1122	0.25	0.1255
O0H	-0.6758	0.312	0.711
H0I	0.4287	0.00	0.00
C0J	0.207	0.35	0.276
O0K	-0.4255	0.29	0.5857
H0M	0.1409	0.25	0.1255
O0N	-0.5498	0.312	0.711
H0O	0.4212	0.0	0.0

Table S2: Atomic charges and non-bonded parameters for SPC/E water molecule.

Atom name	charge	σ (nm)	ε_i (kJ/mol)
OW	-0.8476	0.316	0.65
HW	0.4238	0.000	0.00

Table S3: Atomic charges and non-bonded parameters for urea molecule.

Atom name	charge	σ (nm)	ε_i (kJ/mol)
C	0.124	0.375	0.65898
O	-0.322	0.296	1.31796
N	-0.453	0.355	1.06692
HT	0.276	0.000	0.00000
HC	0.276	0.000	0.00000
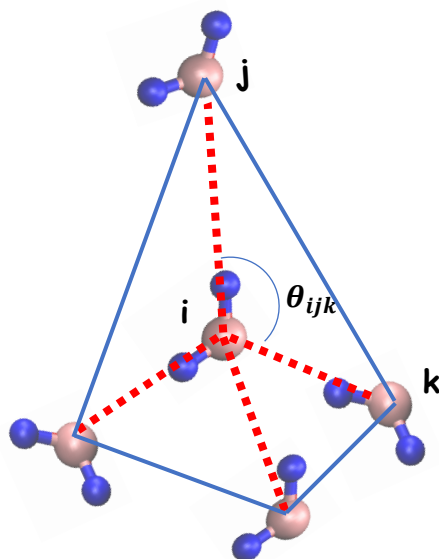
Scheme S2: Schematic representation of water tetrahedral hydrogen bond arrangement. Nearest neighbour water-water-water angle is shown.
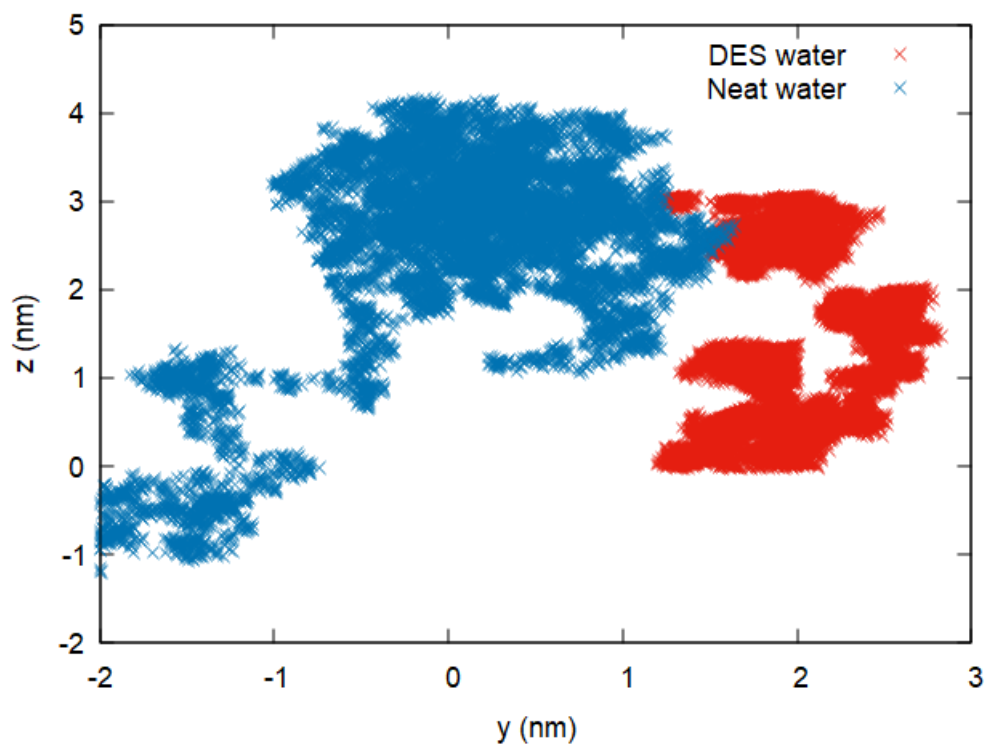
Figure S2: Two-dimensional translational trajectory plot of one random water over 5 ns timespan. Red represent trajectory for DES water while the blue points represent neat water.

Table S4: Multi-exponential fit parameters for continuous water-water H-bond relaxation $(S_{HB}(t))$ in this (glucose+urea+water) DES and in neat water. All the continuous H-bond relaxation functions have been fitted to the equation $f(t) = \sum_{i=1}^{n}[a_i e^{-\frac{t}{\tau_i}}]$.

$S_{HB}(t)$	a_1	τ_1 (ps)	a_2	τ_2 (ps)	a_3	τ_3 (ps)	$< \tau_S^{HB} >$ (ps)
Neat water at 328K	0.1832	0.0934	0.8027	0.4913	--------	--------	0.417
Water in DES	0.1505	0.0827	0.528	0.529	0.322	1.629	0.816

Table S5: Multi-exponential fit parameters for structural water-water H-bond relaxation $(C_{HB}(t))$ in this (glucose+urea+water) DES and in neat water. All the structural H-bond relaxation functions have been fitted to the equation $f(t) = \sum_{i=1}^{n}[a_i e^{-\frac{t}{\tau_i}}]$.

$C_{HB}(t)$	a_1	τ_1 (ps)	a_2	τ_2 (ps)	a_3	τ_3 (ps)	a_4	τ_4 (ps)	$< \tau_C^{HB} >$ (ps)
Neat water at 328 K	0.22	0.32	0.64	2.98	0.14	17.92	--	---	4.51
Water in DES	0.14	0.264	0.12	5.32	0.35	36.63	0.40	346.60	137.11