Supplementary Documents

Enhanced Oil Recovery Promoted by Aqueous Deep Eutectic Solvents on Silica and Calcite Surfaces: A Molecular Dynamics Study

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1. Force-field details of DES molecules

Table S1. Force-field (Non-bonded) parameters of DES and water molecules

Atom name	***Sigma*** (σ) (nm)	***Epsilon*** (ε) $(Kcal/mol)$	q (e^-)
N (Urea)	0.355	0.2550	-0.453
O (Urea)	0.296	0.3150	-0.322
HT (Urea)	0.00	0.00	0.276
HC (Urea)	0.00	0.00	0.276
C (Urea)	0.375	0.1575	0.124
OG (Ethylene glycol)	0.3	0.2975	-0.560
HO (Ethylene glycol)	0.00	0.00	0.348
HG (Ethylene glycol)	0.25	0.0525	0.048
CG (Ethylene glycol)	0.35	0.1155	0.116
CS (Choline)	0.35	0.066	-0.131
HS (Choline)	0.26	0.03	0.068
NA (Choline)	0.325	0.17	0.791

CA (Choline)	0.35	0.066	-0.100
CW (Choline)	0.35	0.066	0.132
OY (Choline)	0.307	0.17	-0.468
HA (Choline)	0.25	0.03	0.033
HW (Choline)	0.22	0.03	0.034
HY (Choline)	0.00	0.00	0.275
Cl (Chloride)	0.377	0.148	-0.800
CT (Menthol)	0.35	0.0783	-0.10
HC (Menthol)	0.25	0.0356	0.05
O (Menthol)	0.312	0.20174	-0.61
HO (Menthol)	0.00	0.00	0.38
Hw (water)	0.00	0.00	0.410
Ow (water)	0.3166	0.1553	-0.820

2. Initial configuration of Confined system with no-DES

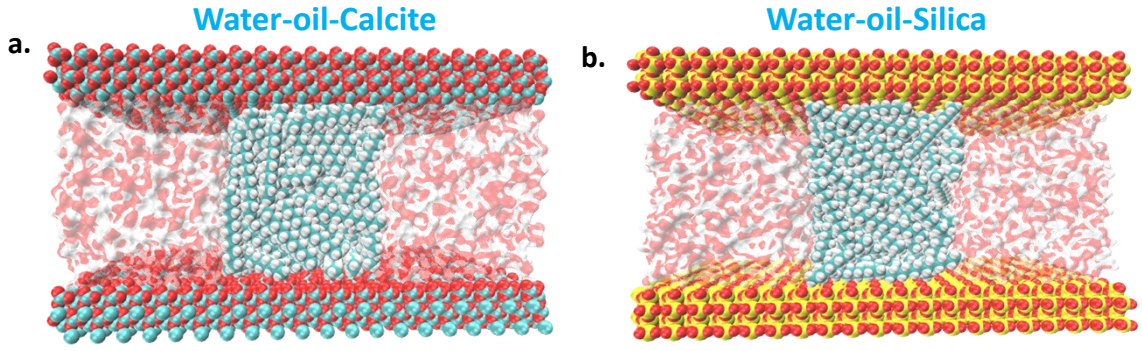


Figure S1. Initial Configuration of systems containing oil molecules with no DES

3. Oil Removal process

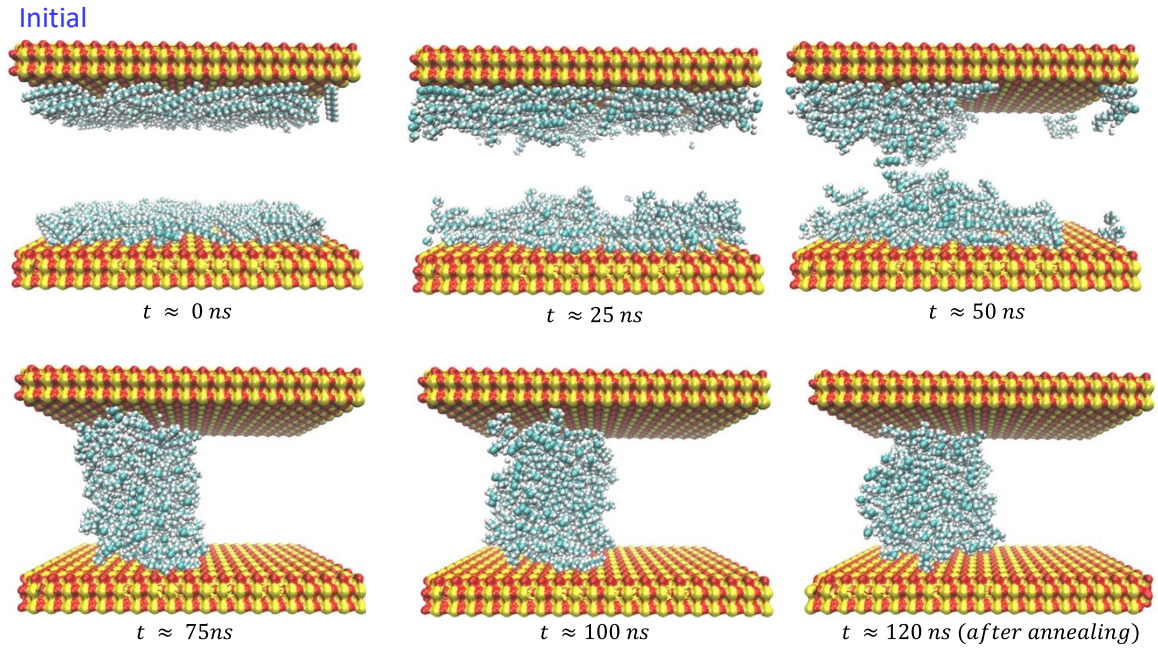


Figure S2. The evolution of the oil layer on the confinement in the presence of water-DES (Water-M:SA) on the SiO_2 surface.

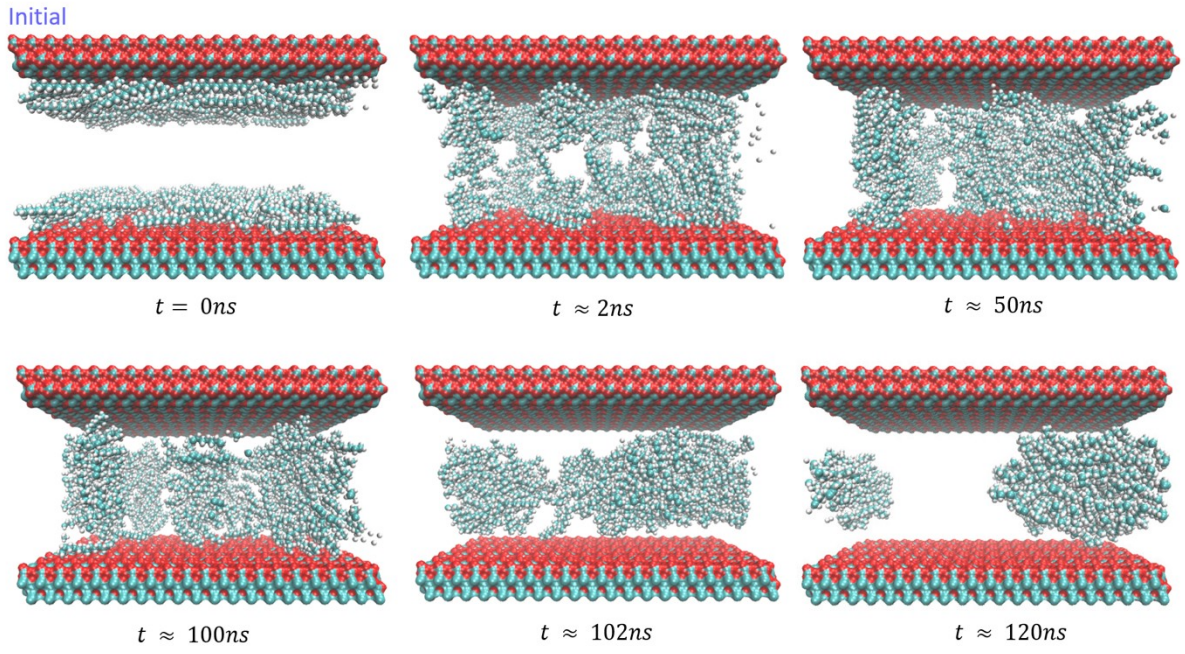


Figure S3. The evolution of the oil layer on the confinement in the presence of water-DES (Water-M:SA) on the $CaCO_3$ surface.

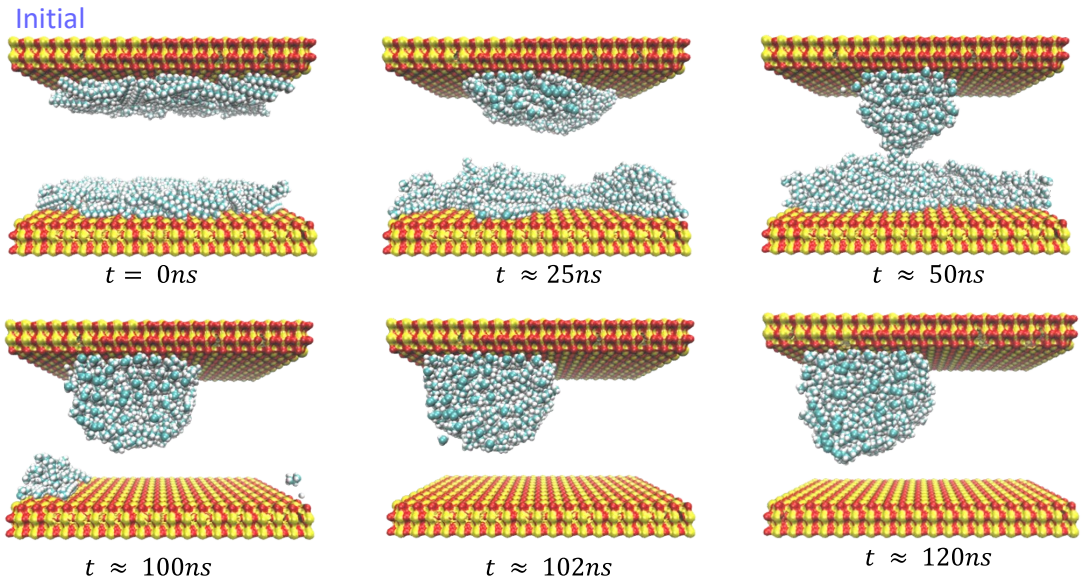


Figure S4. The evolution of the oil layer on the confinement in the presence of water-DES (Water-CCU:EG) on the SiO_2 surface.

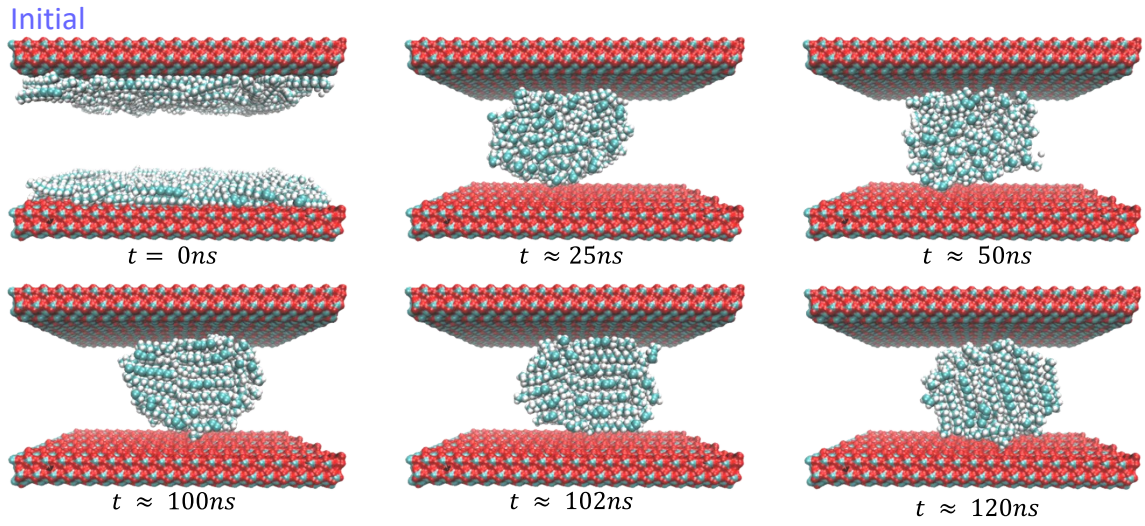


Figure S5. The evolution of the oil layer on the confinement in the presence of water-DES (Water-CCU:EG) on the $CaCO_3$ surface.

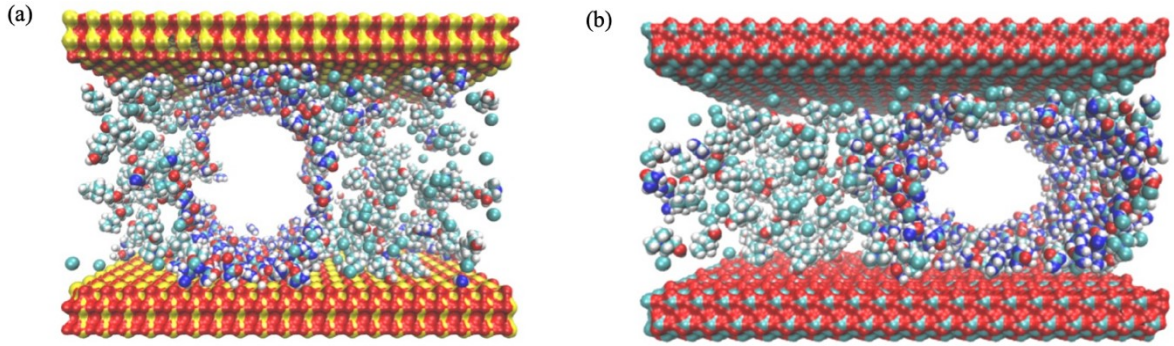
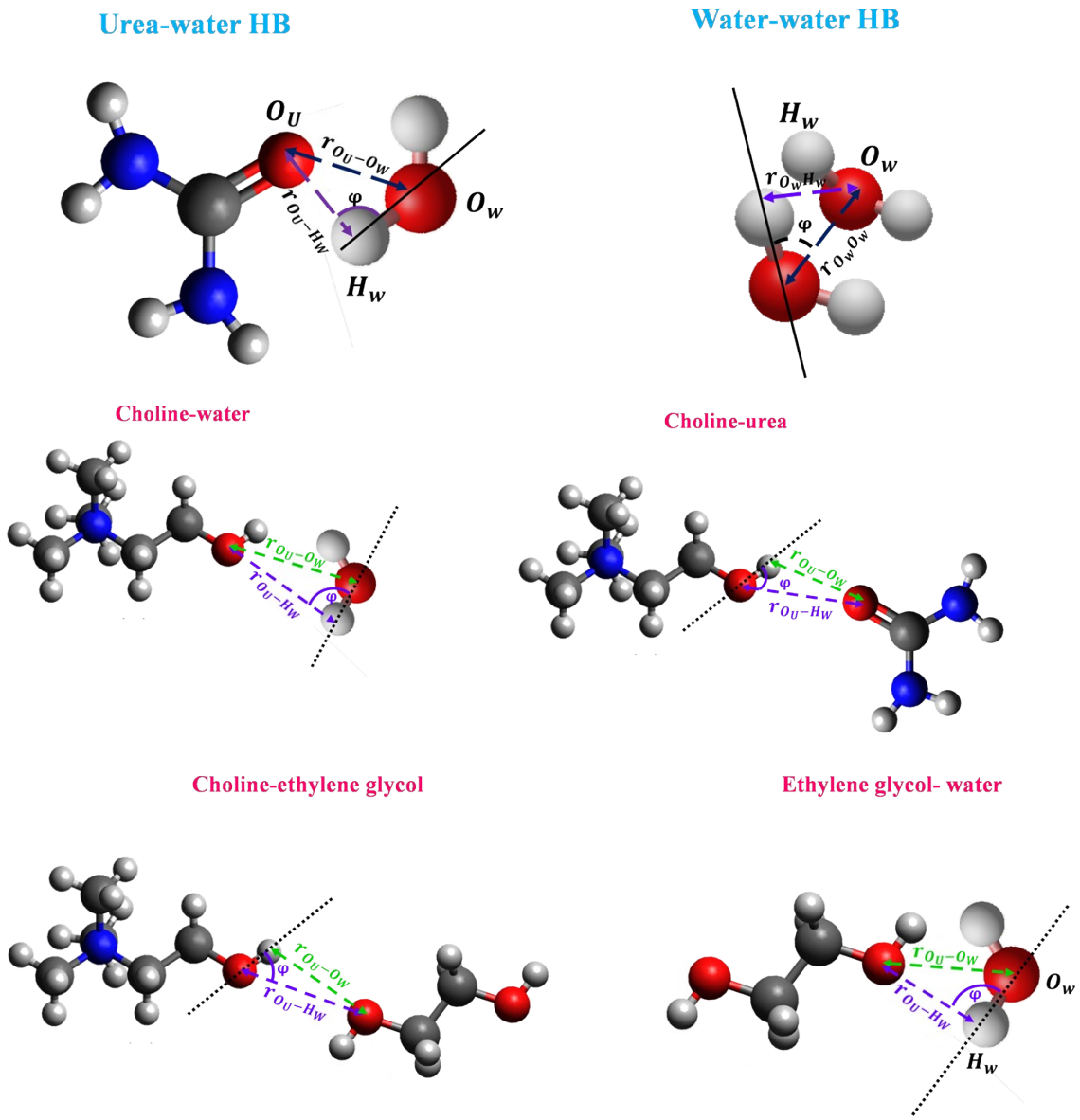


Figure S6. The final configuration shows DES for oil confinement in the vicinity of water-DES (Water-ChCl:U) on the SiO_2 and $CaCO_3$ surfaces.

4. Hydrogen Bonding criteria



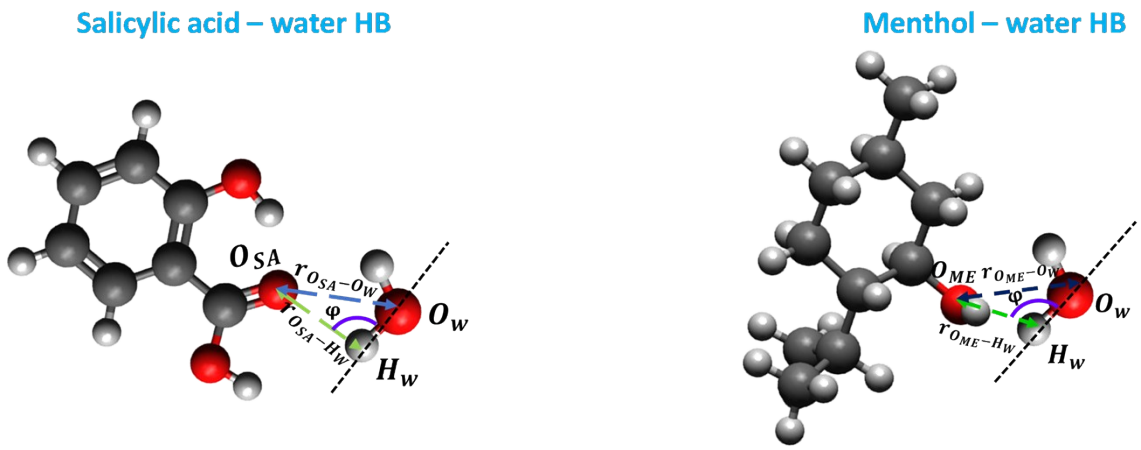


Figure S7. Hydrogen Bonding (HB) between different molecules in DES + Water systems.

Table S2. Geometric criteria for the existence of HB's in aqueous DES systems

Molecule	Acceptor atom	Distance (Å)	Angle (°)
Water	O	3.5	30
Urea (U)	O,N	3.45, 3.5	30
Choline (Ch)	O	3.4	30
Ethylene-glycol (EG)	O	3.5	30
Salicylic acid (Sa)	O	0.35	30
Menthol (ME)	O	0.3	30