Evaluating A Novel Theoretical Strategy for the Screening DES(s) for Potential Application in EOR Processes using Quantum Mechanics Calculations

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Abstract: Green solvents like DES have gained tremendous attention and have been employed for many applications, as industries are now geared towards adopting green materials technologies to contain the effects of climate change, environmental pollution and global warming. They have found application and use in enhanced oil recovery in the petroleum industry as surface active materials, among others. However, there is a need to be able to select, screen and rank the best performance DESs among a large combination of HBA and HBD capable of forming DESs that can perform for enhanced oil recovery (EOR), viz –viz, additional oil recovery. In this study, choline chloride (CHCL) based DESs the most employed DES in EOR are screened for their ability to reduce interfacial tension, adsorption capacities and oil enhancement. We innovate a screening criterion using molecular descriptors obtained from the interaction of the DES with species (rock, water, oil and brine) used in the reservoir. Our findings indicate that the correlation of experimental properties with calculated descriptors can be used to predict the overall EOR performance. Our study contributes to valuable insights into the screening of DESs theoretically to be used for EOR, also can be employed as a quick check to reduce trial and error during the experimental selection of energetically stable DESs in the laboratory for their potential application for EOR performance in a cost-effective manner.

Keywords: Enhanced oil recovery; deep eutectic solvent; quantum chemical; Screening

1. Introduction

DESs is a promising green solvent and have found application in many industries such as pharmaceutical, electrochemical, water treatment, catalysis, and petroleum industries for drilling as shale inhibitors and mud loss control, in flow assurance as wax and asphaltene inhibitors and gas hydrate formation mitigations, and as promising chemicals for enhanced oil recovery as surface active and viscosity modifying agents for interfacial tension reduction and mobility control [1]–[3]. DESs that meet the criteria to be used as EOR agents to recover the residual oil trapped in the reservoir should possess interfacial tension reduction (IFT), wettability alteration, sweep and favorable mobility control properties [4]. The combinations of these properties will result in a better EOR performance for a potential DES. Researchers are in search of a combination of HBA and

HBD that has ability to lower the IFT, and adsorption onto the rock surface and also can increase oil recovery for EOR application.

Mohsenzadeh et al. [5] studied DESs formed using choline chloride with urea and choline chloride with glycerol. The authors reported that the DESs used did not reduce the IFT, but instead, an increase in IFT was obtained. Increase in IFT was reported by Shuwa et al. [6] and with minimal adsorption onto the surface with little possibility of causing formation damage. Al-Wahaibi et al. [7] also reported increased interfacial tension for DESs formed by choline chloride and malonic acid. Lower IFT has been recorded for DESs reported by El-hoshoudy et al. [1] and Hadj-Kali et al. [8], which accounted for the improved oil recovery recorded. Therefore, there is a need to develop a screening strategy that will help screen energetically stable DESs that can perform for EOR. The strategy for building and formation of energetically stable DES from HBA and HBD has been reported in our previous work Uzochukwu et al. [9], which has also been employed in the formation of the DESs used in the screening in this study.

This study presents a unique screening method for easing the selection of DESs for potential application for EOR, using a quantum chemical calculation. This strategy will serve as a quick check and reduce trial and error and material wastage in exploring which combination of HBA and HBD will form an energetically stable DES and their potential capacity for oil enhancement and additional oil recovery.

2. Computational Details

The Spartan v20 molecular modeling package was employed to compute the different levels of computation in our study. Our calculations, we employed the use of density functional theory calculations using B3LYP hybrid functional and 6-31G in the calculations of infrared spectra, electronic energies, and other relevant parameters. A Dell Precision 3520 mobile workstation with a RAM of 24GB, a processor capacity of 7 cores, and a storage capacity of 1TB SSD was used.

3. Results and Discussion

In this study we investigated the interaction involved in the EOR processes, which include oil, brine, rock, and water using quantum chemical calculation. The benzene and pentane were used as model oil, silicate clusters both straight and triangular adopted from literature were used to model the sandstone rock, while sodium chloride was used to model brine. The energetically stable DESs used in the study were built based on a strategy reported in our previous work by Uzochukwu et al. [9]for CHL:GLC,CHL:EGL and CHL:URE [10] . The study evaluated the different deep eutectic solvent formation mechanisms by analyzing different interaction points on HBA (choline chloride; CHL) (Cl, H, O, and N) with HBD (Glycerol, ethylene glycol) on (O, H, and C) with their corresponding formation reaction energy, also known as binding energy. The energies are computed using the expression in Equation 1.

$$BE = E_{des} - E_{HBA} - E_{HBD} \qquad (1)$$

Where E_{des} is the electronic energies of the DES, E_{HBA} is the electronic energies of the hydrogen bond acceptor, and E_{HBD} is the electronic energies of the hydrogen donor. All the electronic energies are collected in eV. The energy that is most exothermic, shown with the highest negative value, would signifies the best and most feasible interaction points.

3.1. Evaluation of DES-oil-rock-water interactions as molecular descriptors for EOR performance

We present the results of the electronic energies of the model species (oil, water, brine rock) used for interaction with DESs to depict different EOR properties and the formation energies of the DESs were computed, which is given in Table 1.
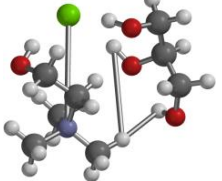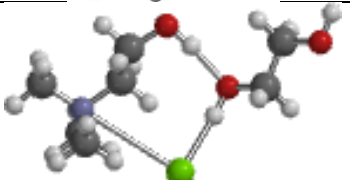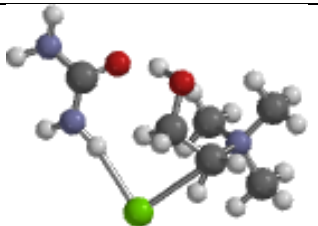
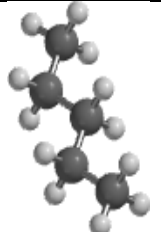*Chem. Proc.* **2022**, *4*, x FOR PEER REVIEW

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From the results presented in Table 1, which show the electronic energies and the most stable geometric structure of the DESs, oil and rock models, and water used in the computation of interactions to depict different mechanisms for oil recovery. It can be seen that among the DESs studied, CHL-GLC was more exothermic and had more negative value, hence more stable, followed by CHL-EGL than CHL-URE DES. For the oil and rock models, the most stable was the pentane and straight silicon oxide cluster.

3.2. Interaction of the reservoir species with DESs using DFT Calculation

The energies of the interaction of these reservoir species: oil, rock, water and brine with the DESs (CHL-EGL, CHL-GLC and CHL-URE) were computed using PM3 level of calculation exploring different point of interactions and the most stable interactions from PM3 were revalidated using DFT. The results are presented in presented in Table 2-7

Analysis of the results shows that the binding energies for the interactions of DES and oil (C5, BZ), DES and rock (Ss and St) and brine and oil, of which the most energetically stable structure are; for the oil model was BZ and for the rock was St. The overall most stable interaction using DFT calculation is presented in Table 8. Both PM3 and DFT level of calculations, similar trend were observed for the interaction of DES and oil (C5, BZ), DES and Rock (Ss and St) and brine and oil with only difference in the magnitude in the binding energies of which their most energetically stable interaction.

Table 1. Electronic energies and structure of relevant species' models.

Descriptions.	Code / Symbol	DFT-E (eV)	Structure
CHL-GLC	OH-H-HO	-30855.21	
CHL-EGL	Cl-HO-H	-27738.32	
CHL-URE	Cl-H	-27603.00	
Silicate (Straight)	Ss	-11971.06	
Silicate (Triangular)	St	-11968.92	
Oil Model (Pentane)	C5	-5381.64	
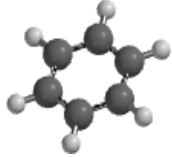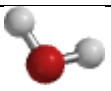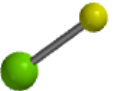
Descriptions.	Code / Symbol	DFT-E (eV)	Structure
Oil Model (Benzene)	BZ	-6319.81	
Water	W	-2079.19	
Sodium chloride (brine)	Br	-16939.80	

Table 2. Interaction of oil (BZ, C5) and rock (Ss, St) with CHL-EGL using PM3.

Label	E (eV)	BE-C5 (eV)	BE-BZ (eV)	BE-Ss (eV)	BE-St (eV)
CHL-EGL[Ss]	-2.52	-	-	-0.02	-
CHL-EGL[Ss][1]	0.11	-	-	2.61	-
CHL-EGL[Ss][2]	5.27	-	-	7.77	-
CHL-EGL[Ss][3]	8.10	-	-	10.6	-
CHL-EGL[St]	0.64	-	-	-	0.39
CHL-EGL[St][1]	-1.78	-	-	-	-2.03
CHL-EGL[St][2]	2.70	-	-	-	2.45
CHL-EGL[St][3]	0.97	-	-	-	0.72
CHL-EGL[C5]	0.05	0.17	-	-	-
CHL-EGL[C5][1]	1.18	1.3	-	-	-
CHL-EGL[C5][2]	2.58	2.7	-	-	-
CHL-EGL[C5][3]	3.84	3.96	-	-	-
CHL-EGL[BZ]	2.31	-	-0.06	-	-
CHL-EGL[BZ][1]	3.7	-	1.32	-	-
CHL-EGL[BZ][2]	5.24	-	2.87	-	-
CHL-EGL[BZ][3]	12.38	-	10	-	-
CHL-EGL[BZ][4]	8.33	-	5.95	-	-
Overall/CHL-EGL	**-**	**0.17**	**-0.06**	**-0.02**	**-2.03**

Table 3. Interaction of oil (BZ, C5), rock (Ss, St), water and brine with CHL-EGL using DFT.

Label	Interact	E (eV)	BE-BZ (eV)	BE-St (eV)	BE-St/BZ (eV)	BE-St/W(eV)	BE-Brine/BZ
CL-HO-H	DES	-27738.32	-	-	-	-	
CL-HO-H[BZ]	DES-BZ	-34058.13	0.00	-	-	-	
SiO2s	Ss	-11971.06	-	-	-	-	
SiO2t	St	-11968.92	-	-	-	-	
C5	C5	-5381.64	-	-	-	-	
SiO2t[BZ]	St-BZ	-18288.69	-	-	0.05	-	
benzene	BZ	-6319.81	-	-	-	-	
water	W	-2079.19	-	-	-	-	
NaCl	brine	-16939.80					
St[water][3]	Ss-W	-14048.52	-	-	-	-0.41	
NaCl[BZ]	Brine-BZ	-23257.02					-0.58
CL-HO-H[St][1]	DES-St	-39708.52	-	-1.28	-	-	

Table 4: Interaction of oil (BZ, C5) and rock (Ss, St) with CHL-GLC using PM3.

Label	E (eV)	BE-C5 (eV)	BE-BZ (eV)	BE-Ss (eV)	BE-St (eV)
CHL-GLC[Ss]	-8.08	-	-	0.63	-
CHL-GLC[Ss][1]	-1.94	-	-	6.76	-
CHL-GLC[Ss][2]	-4.82	-	-	3.89	-
CHL-GLC[Ss][3]	-4.89	-	-	3.82	-
CHL-GLC[St]	-6.13	-	-	-	-0.17
CHL-GLC[St][1]	-4	-	-	-	1.96
CHL-GLC[St][2]	-5.53	-	-	-	0.42
CHL-GLC[St][3]	-2.6	-	-	-	3.36
CHL-GLC[C5]	-6.74	-0.42	-	-	-
CHL-GLC[C5][1]	-5.68	0.65	-	-	-
CHL-GLC[C5][2]	-4.94	1.38	-	-	-
CHL-GLC[C5][3]	-5.09	1.24	-	-	-
CHL-GLC[BZ]	-4.35	-	-0.52	-	-
CHL-GLC[BZ][1]	1.89	-	5.72	-	-
CHL-GLC[BZ][2]	-3.44	-	0.39	-	-
CHL-GLC[BZ][3]	4.61	-	8.44	-	-
Overall	**-**	**-0.42**	**-0.52**	**0.63**	**-0.17**

Table 5: Interaction of oil (BZ, C5), rock (Ss, St), water and brine with CHL-GLC using DFT.

Label	Interact	E (eV)	BE-BZ (eV)	BE-St (eV)	BE-St/BZ (eV)	BE-St/Water (eV)	BE-Brine/BZ
OH-H-HO[St]	St	-42825.3	-	-1.17	-	-	-
OH-H-HO	des	-30855.21	-	-	-	-	-
OH-H-HO[BZ]	BZ	-37175.18	-0.16	-	-	-	-
SiO2s	Ss	-11971.06	-	-	-	-	-
SiO2t	St	-11968.92	-	-	-	-	-
C5	C	-5381.64	-	-	-	-	-
benzene	BZ	-6319.81	-	-	-	-	
water	W	-2079.19	-	-	-	-	-
SiO2t[benzene]	St-BZ	-18288.69	-	-	0.05	-	-
SiO2t[water][3]	Ss-W	-14048.52	-	-	-	-0.41	-
NaCl	brine	-16939.80	-	-	-	-	-
NaCl[BZ]	Brine-BZ	-23257.02	-	-	-	-	-0.58

Table 6: Interaction of oil (BZ, C5) and rock (Ss, St) with CHL-URE using PM3.

Label	E (eV)	BE-C5 (eV)	BE-BZ (eV)	BE-Ss (eV)	BE-St (eV)
CHL-URE[Ss]	-0.88	-	-	1.44	-
CHL-URE[Ss][1]	3.56	-	-	5.88	-
CHL-URE[Ss][2]	-1.67	-	-	0.65	-
CHL-URE[Ss][3]	3.25	-	-	5.57	-
CHL-URE[Ss][4]	5.1	-	-	7.42	-
CHL-URE[Ss][5]	2.6	-	-	4.92	-
CHL-URE[St]	0.3	-	-	-	-0.13
CHL-URE[St][1]	-0.65	-	-	-	-1.08
CHL-URE[St][2]	0.53	-	-	-	0.1
CHL-URE[St][3]	2.82	-	-	-	2.38
CHL-URE[C5]	0.05	-0.01	-	-	-
CHL-URE[C5][1]	2.29	2.23	-	-	-
CHL-URE[C5][2]	1.04	0.98	-	-	-
CHL-URE[C5][3]	3.1	3.04	-	-	-
CHL-URE[BZ]	2.53	-	-0.03	-	-
CHL-URE[BZ][1]	5.17	-	2.62	-	-
CHL-URE[BZ][2]	3.59	-	1.03	-	-
CHL-URE[BZ][3]	8.74	-	6.18	-	-
CHL-URE[BZ][4]	11.43	-	8.87	-	-
Overall	**-**	**-0.01**	**-0.03**	**0.65**	**-1.08**

Table 7. Interaction of oil (BZ), rock (St) with CHL-URE (Cl-H) using DFT.

Label	Interact	E (eV)	BE-BZ (eV)	BE-St (eV)	BE-St/BZ (eV)
Cl-H[St][1]	St	-39573.28	-	-1.36	-
Cl-H	DES	-27603	-	-	-
Cl-H[BZ]	B	-33922.91	-0.1	-	-
SiO2t	St	-11968.92	-	-	-
benzene	BZ	-6319.81	-	-	-
SiO2t[BZ]	St-B	-18288.69	-	-	0.05

Table 8. Overall binding energies of oil, DES and rock using DFT Calculation.

DES	DES/Oil (eV)	St/Oil (eV)	DES/St (eV)	W/St (eV)	St /DES (eV)	Oil/St (eV)	DES/Oil (eV)	Oil/brine (eV)
CHL-URE	-0.10	0.05	-1.36	-0.41	-1.36	0.05	-0.16	-0.58
CHL-GLC	-0.16	0.05	-1.17	-0.41	-1.17	0.05	0	-0.58
CHL-EGL	0.00	0.05	-1.28	-0.41	-1.28	0.05	-0.1	-0.58

Table 9. Molecular relations accounting for different behaviors' in EOR processes from DFT.

DES	DES/Oil>St/Oil	DES/St<W/St	St/DES>Oil/St	DES/oil< oil/brine
CHL-URE	-0.10 >0.05	-1.36>-0.41	-1.36>0.05	-0.1<-0.58
CHL-GLC	-0.16 >0.05	-1.17>-0.41	-1.17>0.05	-0.16 < -0.58
CHL-EGL	0.00>0.05	-1.28>-0.41	-1.28>0.05	0 < -0.58

Table 10. Experimental data obtained from literature for EOR performance.

DES	EXPT.IFT(mN/m)	EXPT.ADS (mg/g)	EXPT.AOR(%)	Reference
CHL-URE	4.3	9.5	25	[1]
CHL-GLC	1.52	10.5	22	[1]
CHL-EGL	5	8.5	15	[1]

3.3. Screening of the different DESs for EOR Applications

In this section we explore the use of descriptors like DES/Oil>St/Oil [ease of emulsification of the oil by DES and or the ease of breaking the adhesive force between the oil and rock]; DES/St>Oil/St [sweeping efficiency or wettability] and DES/Oil>brine/Oil [ease of interfacial tension reduction] (Table 9) to evaluate for possible correlation with the experimental result for IFT, DES adsorption, and AOR in the literature (see Table 10).

Using the molecular relationships for the interactions presented in Table 3, the relations were simplified by normalizing the molecular descriptors using Equations 2-5. To facilitate equal weight averaging of the overall contributions of indicators accounted by each of the descriptors, the molecular descriptors were further normalized to obtained values within 0-1, where descriptors having negative values were normalized using equation 7 and those with positive values calculated using Equation 6 and this result presented in Table 12.

Table 11. Molecular descriptors accounting for different behaviors in EOR processes.

DES	DES/oil > St/oil	DES/St < W/St	DES/St > St/oil	DES/oil < brine/oil
CHL-URE	3.00	-2.32	28.20	0.83
CHL-GLC	4.20	-1.85	24.40	0.73
CHL-EGL	1.00	-2.12	26.60	1.00
SUM	8.20	-6.29	79.20	2.55

Table 12. Normalized molecular descriptors and averaged-descriptors accounting for overall behavior.

DES	DES/oil > St/oil	DES/St < W/St	DES/St > St/oil	DES/oil < brine/oil	AVG-RECOVERY
CHL-URE	0.37	0.32	0.36	0.32	0.34
CHL-GLC	0.51	0.35	0.31	0.28	0.36
CHL-EGL	0.12	0.33	0.34	0.39	0.30
SUM	1.00	1.00	1.00	1.00	1.00

The correlation of these results with experimental results is presented in Table13, which would facilitate the ease of identifying the best descriptors for IFT, adsorption, and AOR.

Table 13. Correlation coefficient of experimental properties with calculated descriptor.

	EXPT.IFT	EXPT.ADS	EXPT.AOR	
AVG/X	-0.87	0.98	0.80	AVG
COL1/X	-0.89	0.99	0.78	d/oil > s/oil
COL2/X	-0.81	0.58	-0.20	d/s < w/s
COL3/X	0.81	-0.58	0.20	d/s > s/oil
COL4/X	0.89	-0.99	-0.78	d/oil < b/oil

$$D_1 = I_{DOIL-SOIL} = \frac{SOIL-DOIL}{SOIL} \quad (2);$$

$$D_2 = I_{DS-WS} = \frac{WS-DS}{WS} \quad (3);$$

$$D_3 = I_{DS-SOIL} = \frac{SOIL-DS}{SOIL} \quad (4);$$

$$D_4 = I_{DOIL-BOIL} = \frac{BOIL-DOIL}{BOIL} \quad (5);$$

$$N_{DOIL-SOIL} = \frac{I_i}{\sum I_i} \quad (6);$$

$$N_{DS-SOIL} = 0.5 - 0.5 \frac{I_i}{\sum I_i} \quad (7)$$

Where DOIL= DES/oil; SOIL = St/oil; BOIL= brine/oil; WS = W/St; DS = DES/St interactions, IFT= interfacial tension reduction, ADS= adsorption and AOR= additional oil recovery.

From Table 7, it can be seen that from the correlation of experimental data with the calculated descriptor DES/Oil > St/oil (R=-0.89) and DES/Oil St/oil (R=0.99) and DES/oil < brine/oil (R=-0.99) approximately would be best predict adsorption, while the best descriptor for the AOR was found to be overall average (R=0.8). However, there are efforts to employ the use of other methods for systematically averaging the overall properties contribution is being investigated to obtain the best descriptor for the AOR since it is the goal for EOR.

4. Conclusions

This study successfully developed a screening strategy for Deep Eutectic Solvents (DESs) that can be used to enhance oil recovery. The strategy is based on the molecular descriptors calculated from the binding/adsorption energies between the DES and oil, DES and rock, oil and rock, water and rock, and brine and oil. Our study reveal that when screening DESs for IFT reduction, when the binding strength of DES/Oil > St/oil and DES/Oil<brine/oil molecular descriptor are most suitable, DES/Oil > St/oil and DES/oil < brine/oil would be best predict adsorption and DES/Oil > St/oil and DES/Oil<brine/oil were most predict AOR with an approximate correlation coefficient of 0.8.

The results of our study demonstrate that molecular descriptors can be used to predict and screen DESs for Enhanced Oil Recovery (EOR) applications. Finally, we recommend the use of this screening strategy to select thermodynamically stable DESs for EOR.

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