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Integrated DFT Study of CO_2 Capture and Utilization in Gingerol Extraction Using Choline Chloride–Lactic Acid Deep Eutectic Solvent

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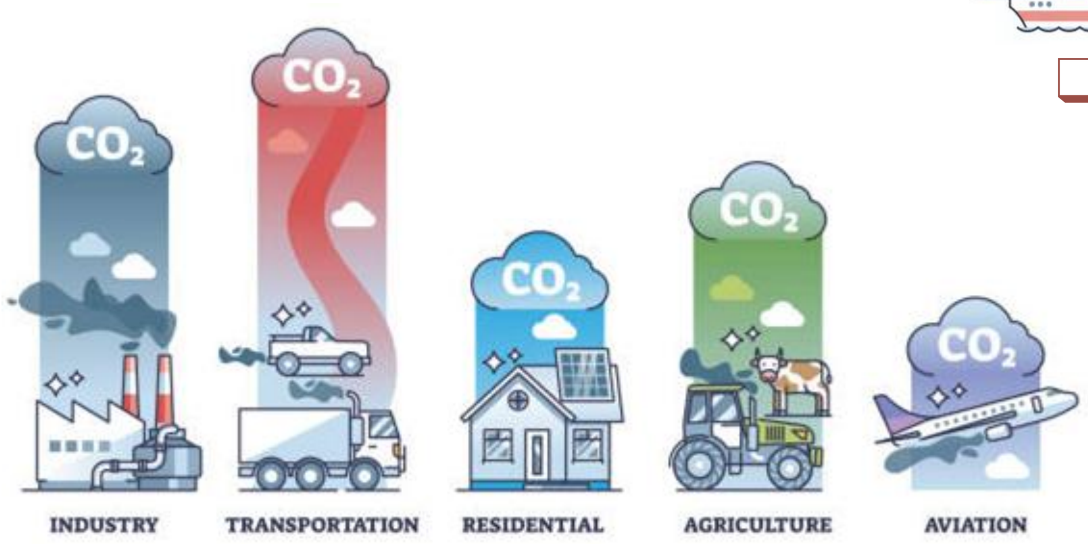
INTRODUCTION & AIM

- ❑ The rate of carbon emission has continued to be subject of concern global due to its larger relative to other greenhouse gases [1,2].

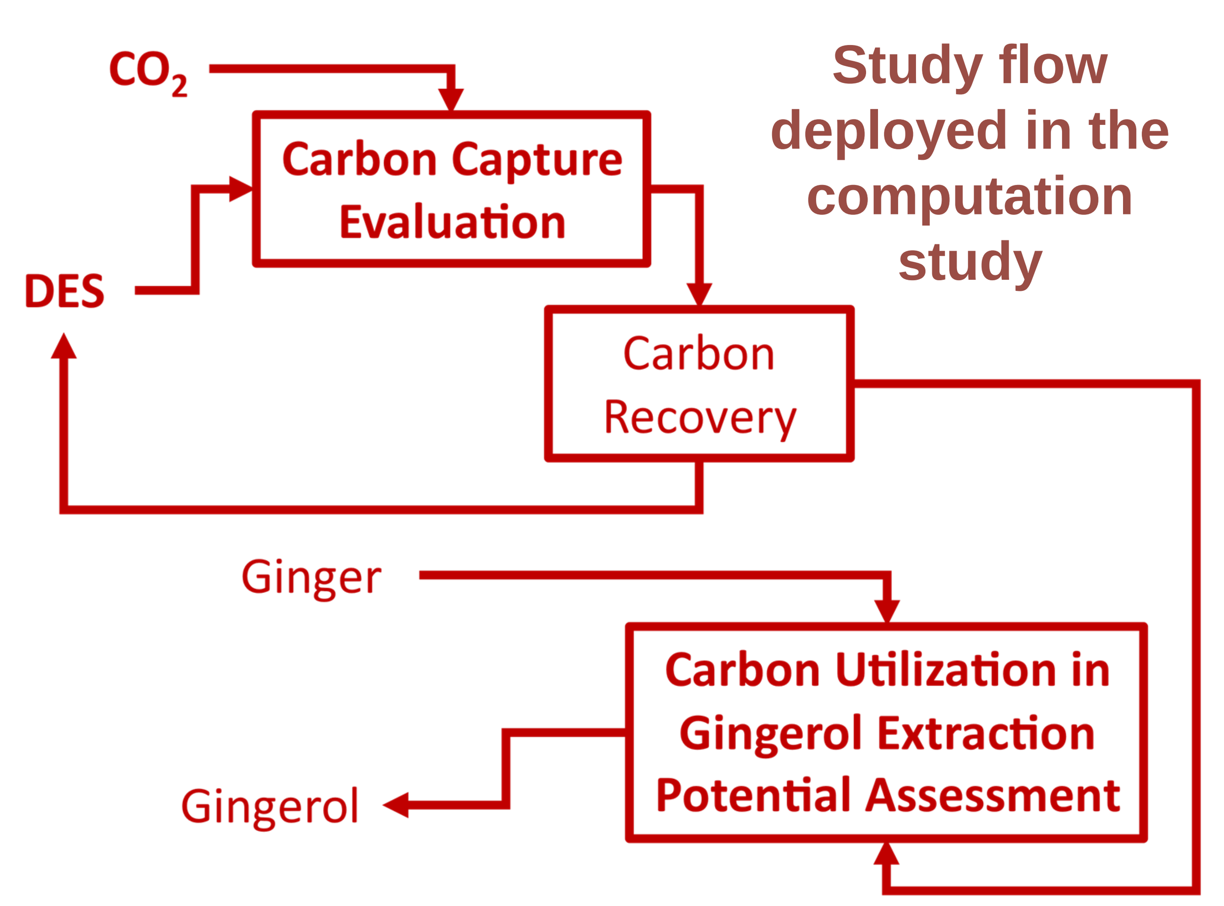


- ❑ It is commonly released through different processes holding in industries, residential places, transportation, and many others [2].

Aim of Study:

To investigate, using DFT, how choline chloride–lactic acid DES captures CO_2 and uses it to enhance gingerol extraction for sustainable pharmaceutical applications.

METHOD



Study flow deployed in the computation study

Computational Resource:
Student Spartan v9

Computational Detail:

Density Functional Theory (DFT) calculation [3] with the wB97X-D functional, and 6-31G(D) [3-21G(*)] basis set starting from PM3-optimized geometries, with a dual basis approach in the gas phase to account for dispersion error.

RESULTS & DISCUSSION

Table 1: Evaluation of DES Formation Energy & HBA-HBD Interaction

DES Component	Molecular Formula	HOMO (eV)	LUMO (eV)	Egap (eV)	IEG-CHL HOMO (eV)	IEG-CHL LUMO (eV)	F.E (eV)
CHL	$C_5H_{14}ClNO$	-7.83	3.04	10.87	10.87	10.87	-1.92
LAC	$C_3H_6O_3$	-10.18	0.99	11.17	8.82	13.22	-1.92

- ❑ **ClC–LAC forms a stable DES (F.E = –1.92 eV) with ClC as the reactive acceptor and LAC as the stable donor.**

- ❑ **The CLC-LAC has a lower energy band gap (11.04 eV) than MEA (12.42 eV), indicating higher chemical reactivity and better suitability for CO_2 capture.**

Table 2: Molecular Properties for Carbon Capture

Species	Molecular Formula	HOMO (eV)	LUMO (eV)	Egap (eV)	IEG-CO_2 HOMO (eV)	IEG-CO_2 LUMO (eV)
CO_2	CO_2	-13.13	1.85	14.98	14.98	14.98
MEA	$C_3H_7NO_3$	-8.80	3.62	12.42	16.75	10.64
CHL-LAC	$CO_2.C_8H_{20}ClNO_4$	-9.34	1.71	11.04	14.83	11.19

Table 3: Carbon Capture Potential of Different Solvents

Solvent	Molecular Formula	Binding Energy (eV)
MEA	$C_3H_7NO_3$	-0.234
CHL-LAC	$C_8H_{20}ClNO_4$	-0.86

- ❑ **DES–CO_2 binding energy (–0.86 eV) is stronger than with MEA (–0.234 eV), indicating better CO_2 capture.**

- ❑ **CO_2–gingerol shows moderate binding (-0.17 eV), suggesting extraction potential.**

- ❑ **DES–gingerol binding is much stronger (-1.87 eV), confirming its effectiveness as a green solvent.**

Table 4: Potential of CO_2 for Gingerol Extraction

DES Component	HOMO (eV)	LUMO (eV)	Egap (eV)	IEG-GIN HOMO (eV)	IEG-GIN LUMO (eV)	B.E (eV)
CO_2	-13.13	1.85	14.98	10.55	10.55	-0.17
GIN	-8.70	0.77	9.48	9.48	9.48	N/A
Ethanol	-9.77	4.28	14.05	12.98	10.55	-0.73
CHL-LAC	-9.34	1.70	11.05	10.10	10.12	-1.87

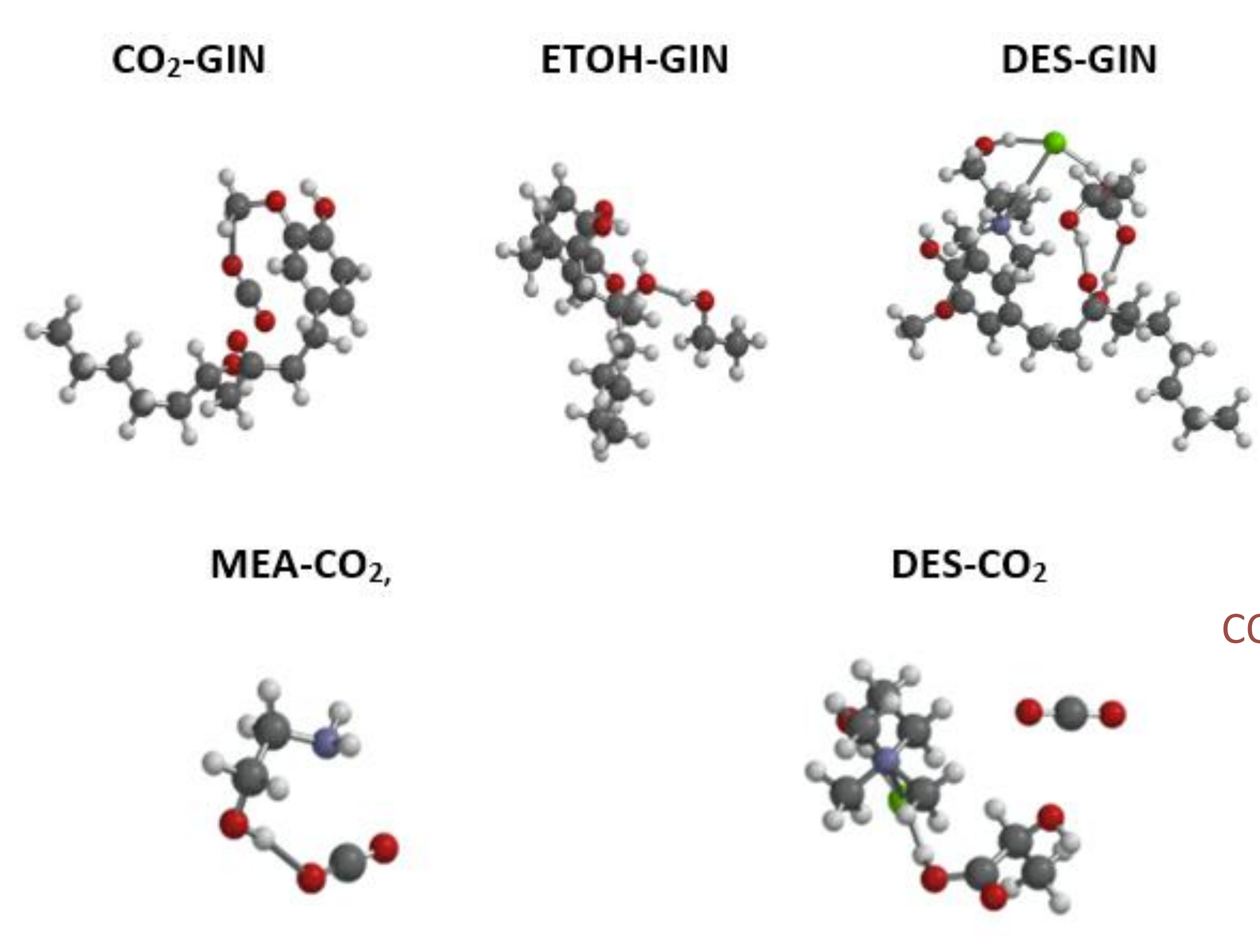


Fig. 1: Most stable geometry structures of CO_2-GIN, ETOH-GIN, MEA-CO_2, , DES-GIN and DES-CO_2 interactions.

CONCLUSIONS

- ❑ CLC-LAC demonstrated stronger CO_2 affinity than MEA, confirming its effectiveness for carbon capture.
- ❑ CLC-LAC high binding energy with 6-gingerol supports its dual use in CO_2 reuse and green pharmaceutical extraction.

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