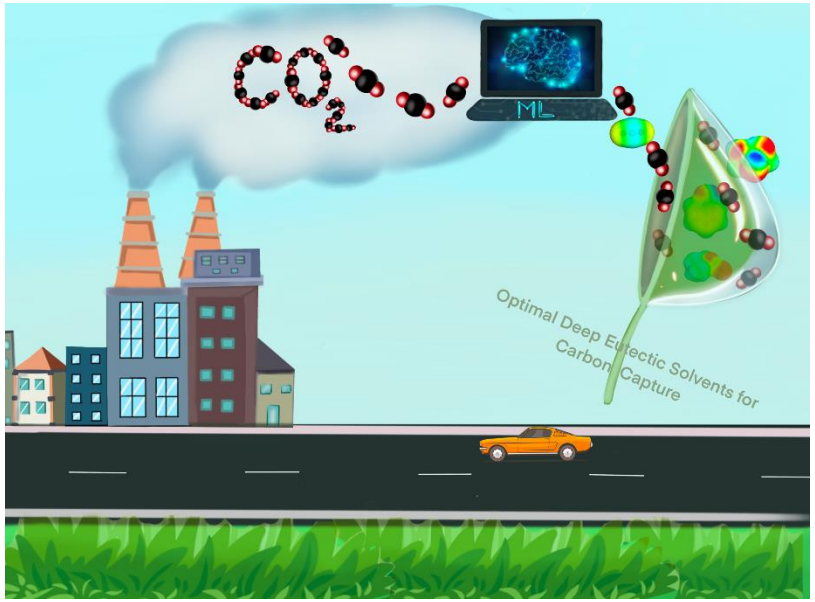
Artificial Intelligence Predicts Carbon Capture in Green Solvents



Schematic diagram for CO2 release and capture using the ML-screened optimal deep eutectic solvents.

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Scientific Achievement

We have shown that the charge polarization at the molecular surface obtained from a quantum chemical calculation (i.e., the COnductor-like Screening MOdel for Realistic Solvents [COSMO-RS]) can be used to train machine-learning (ML) regression models that accurately predict the carbon dioxide (CO_2) solubility of Deep Eutectic Solvents (DESs).

Significance and Impact

ML approaches to predict the solubility of gases in green solvents can reduce the need for expensive and time-consuming experimental solvent screening campaigns in climate change research. Here, we demonstrate that features derived from a computationally inexpensive quantum chemical calculation combined with ML yield models of unprecedented accuracy for CO_2 solubility predictions. These results support our ongoing efforts to apply ML approaches for solvent-based biomass pretreatments — ionic liquids at JBEI and organosolv at ORNL.

Research Details

- A comprehensive dataset of 1,973 data points was collected from the literature on the solubility of CO_2 in 132 different physical-based DESs (molar ratios varying from 1:1 to 1:16) covering a wide range of temperatures and pressures.
- We calculated the probability distribution of charge polarization at the molecular surface for all the DESs molecules, which we hypothesized can implicitly capture intermolecular interactions relevant to solubility. Importantly, these ML features do not require computationally expensive modeling of the intermolecular complex.
- We trained four ML models to predict the CO_2 solubility in DESs. A fully connected neural network model with a single hidden layer had the best predictive performance.
- The ML models developed here more accurately predict CO_2 solubilities in DESs than those previously reported in the literature and can therefore be useful tools for designing and selecting DESs for CO_2 capture.