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Accelerated Discovery of Carbon Capture Solvents

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PURPOSE OF THE ABSTRACT

Carbon capture is part of the road-map towards net zero for many countries around the world, since emissions from existing infrastructure are close to estimated carbon budgets.[1, 2] To address this problem, 87 carbon capture projects are proposed worldwide in the next 10 years.[3] A major class of commercial carbon capture technology involves solvents capture systems. Commonly solvent capture systems feature solvents. These solvents suffer from problems such as degradation, corrosion, and effectiveness. Systematic approaches to improve on the current technology are now needed with increasing urgency to expedite the introduction of cutting-edge carbon capture methods.

In our work we have curated information from the literature related to existing carbon capture solvents. Using this experimental data, we have developed an end-to-end solvent discovery pipeline. Using cloud-based, containerized, computational chemistry workflows, we have built models to assist in the screening of carbon capture solvents. These models utilize a range of computational techniques to ascertain the likely utility of a solvent towards carbon capture. Following screening, we identify promising candidates and complete our end-to-end cycle with laboratory investigations and validation. Experimental validation data are then delivered back to the model to improve its predictive capabilities. The end goal is to identify and generate new solvent candidates with improved performance for carbon capture.

FIGURES

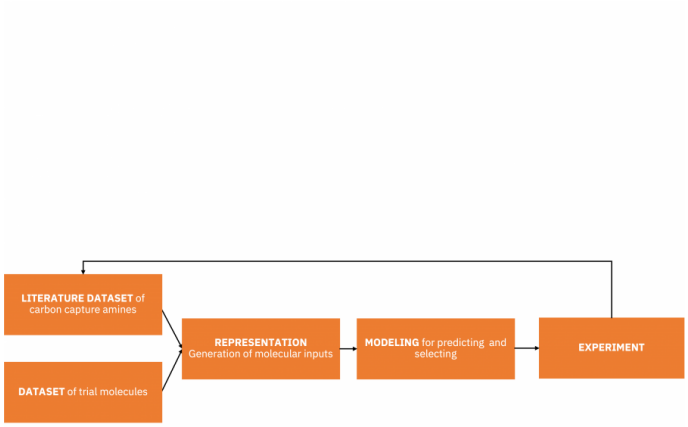

FIGURE 1
Discovery cylce
High level discovery pipeline

FIGURE 2

KEYWORDS
Solvents | carbon capture | discovery | machine learning

BIBLIOGRAPHY