Synthesis and Characterization of Property-Optimized Ionic Liquid for Post-Combustion Carbon Capture Discovered via Novel Deep Learning Model

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Post-Combustion Carbon Capture (PCC) aims to mitigate rising greenhouse gas emissions by sequestering CO2 from flue gas streams. Currently, PCC utilizes liquid amine solvents, such as monoethanolamine, which encounter various chemical drawbacks—including corrosivity, volatility, flammability, and toxicity—that hinder functional and economic efficiency. Ionic Liquids (ILs) have been identified as promising alternative solvents, possessing numerous properties ideal for the process. However, ILs face a comparatively smaller set of energy and efficiency-based challenges that must be overcome prior to PCC implementation. To address these issues, property-optimized ILs with minimal viscosity, minimal heat capacity, and maximal thermal conductivity were designed via a novel generative autoencoder-based deep learning framework in this study. These ILs were analyzed for synthetic cost and feasibility along with theoretical carbon dioxide uptake; an imidazolium-based IL emerged as an ideal compound matching all criteria. A cost and time-effective synthesis process was established, circumventing the inefficient ion-exchange metathesis step typical in IL synthesis. Experimental measurements of the aforementioned properties confirmed the novel IL compound to have substantial energy and efficiency-related improvements over all existing ILs for the PCC process. Moreover, carbon dioxide uptake was quantified, achieving a 1:0.39 molar ratio of solvent to carbon dioxide--a capture rate similar to industry-leading solvents. It was calculated that the optimal IL would reduce energy consumption and cost by at least 34%. These results prove the efficacy of the property-optimizing model and mark a significant leap toward feasible large-scale carbon capture implementation.

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