

A NOVEL CO₂ SEQUESTRATION SYSTEM FOR ENVIRONMENTALLY PRODUCING HYDROGEN FROM FOSSIL-FUELS

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ABSTRACT

Aqueous monoethanolamine (MEA) scrubbers are currently used to capture carbon dioxide (CO₂) from industrial flue gases in various fossil-fuel based energy production systems. MEA is a highly volatile, corrosive, physiologically toxic, and foul-smelling chemical that requires replacement after 1000 operational hours. Room temperature ionic liquids (RTILs), a novel class of materials with negligible vapor pressures and potentiality as benign solvents, may be the ideal replacement for MEA. *Ab initio* computational modeling was used to investigate the molecular interactions of ILs with CO₂. The energetic and thermodynamic parameters of the RTILs as CO₂ solvents are on par with MEA. As viable competitors to the present CO₂ separation technology, RTILs may economize the fossil-fuel decarbonization process with the ultimate aim of realizing a green hydrogen economy.

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