

Discovering direct air capture materials using computational modelling

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Abstract:

Main text: Direct Air Capture (DAC) of carbon dioxide from the atmosphere has become an urgent response tool to balance the global CO₂ concentrations. Performance and scalability are intimately linked as the size and energy consumption greatly depend on the CO₂ capacity and regenerability of the core capture material. The materials are categorized as liquid solvents, solid sorbents and membranes. In this paper, the team will present results from two studies. The first study is analyzing over 200 polymers in the MSA membrane database to identify potential candidates for DAC connected to algae farms and greenhouses. The second study is using a combination of molecular simulation and machine learning to identify metal-organic frameworks (MOFs) capable of capturing large amounts of CO₂ in atmospheric conditions.

Keywords: direct air capture, carbon dioxide, membrane database, molecular simulation, machine learning.

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