

MDLab: AI frameworks for Carbon Capture and Battery Materials

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Background/Objectives. Practical applications of carbon capture by sorbents and membranes require broad knowledge of chemical and material properties and process costs. Appropriate solvents must have high CO₂ capacity and low regeneration energy to be cost effective in operation, and they also need good material properties such as low viscosity and foaming for cyclic motions in a capture plant, low corrosiveness in the plant environment and slow degradation over time. Solid adsorbents and membranes need high capacity and low regeneration energy too, but also high selectivity for CO₂ over other molecules such as N₂ and H₂O. Membranes require high permeability and high selectivity, in addition to material strength. Similarly for battery applications, the chemical and materials properties of electrolytes are increasingly important as the storage industry scales up.

Approach/Activities. IBM's MDLab is a software stack for Materials Discovery that uses AI to screen for carbon capture and battery materials based on measured and computed properties. Techniques include MACCS and other fingerprinting and Mordred descriptors for solvents and electrolytes, geometric and topological descriptors with Grand Canonical Monte Carlo (GMGC) simulations for porous solids, and various machine learning models applied to SMILES encoding of polymer membranes with validation from Classical Molecular Dynamics simulations.

Results/Lessons Learned. Carbon capture amines are found to inhabit an edge region of chemical space, suggesting possible new amines suitable for carbon capture. Certain chemical functional groups are also found to be relatively less common in carbon capture amines compared to other amines, possibly indicating detrimental impact on performance. For nanopore materials screening, geometric and topological descriptors, combined with GCMC simulations, can be compared with measured adsorption properties to rule out unfavorable structures. Predicted new polymer membranes based on extrapolated properties of known membranes were tested computationally with 800 heavy atoms per polymer chain and 6 nm membrane thickness. The resulting CO₂ permeability is the same order as the predicted value. Machine Learning models for high-throughput screening of electrolyte materials based on physico-chemical properties reduce the experimentation needed to find safer and higher performing batteries.

Sample publications:

O'Conchuir et al. 2022 ACS Fall Meeting <https://research.ibm.com/publications/effect-of-partial-charges-on-the-data-driven-analytics-of-co2-adsorption-metrics>

Hsu, H. et al. 2022, APS March Meeting <https://research.ibm.com/publications/computational-design-and-validation-of-polymer-membranes-with-high-co2-permeability>

Luan, B. et al. 2022 APS March Meeting <https://research.ibm.com/publications/the-role-of-partial-charges-in-data-driven-analytics-of-gas-adsorption-simulations>

Mcdonagh, J. et al. 2022 ChemRxiv <https://research.ibm.com/publications/chemical-space-analysis-and-property-prediction-for-carbon-capture-amine-molecules>