ACCELERATED MATERIALS DESIGN FOR CARBON CAPTURE USING ATOMISTIC AND DATA DRIVEN MODELLING INTEGRATED WITH INDUSTRIAL SCALE PROCESS SIMULATIONS

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Metal organic frameworks (MOFs) are crystalline, nanoporous inorganic-organic materials that have attracted significant attention as solid sorbants for various gas separation applications such as large scale CO_2 capture. These materials present an almost infinite design space with innumerable combinations of inorganic and organic building units that can combine to form a permanently porous material. In this presentation, we discuss how data driven modelling has been used to design new materials for post-combustion CO_2 capture that have been realized experimentally and shown to outperform existing materials.[1] We additionally discuss our efforts to integrate atomistic simulations of materials with sophisticated process simulations of the CO_2 capture process[2] with the goal of rationally design materials at the molecular level that are optimized for the industrial process they are to be used in.

REFERENCES

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