Discovering Materials to Stop Climate Change using Molecular Simulations

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Among the many strategies to combat climate change, one is to capture and store the CO_2 that is generated by fossil fuel-based power plants. However, we have yet to find a porous material that can capture CO_2 efficiently - so that the power plant does not need to spend a large fraction of its energy running the CO_2 capture process itself.

Fortunately, in the last decade, a wealth of novel porous crystalline materials have been synthesized by what has come to be called "modular" or "reticular chemistry". This new approach, as opposed to serendipitous methods of the past, leverages the self-assembly of modular molecular "building blocks" that can only assemble in very specific orientations and allows one to design an enormous number of new crystals, far beyond what can actually be synthesized in a reasonable amount of time.

In this work, we present a recently published approach of enumeratively generating all of the hypothetical MOFs (a class of porous crystals) that can be made from a library of modular building blocks. Additionally we demonstrate how this computational approach has been used to identify optimal MOFs that have the highest natural gas storage capacity, as well as the best "selection parameter" (an aggregate of relevant performance metrics) for capturing and storing CO_2. While in many cases the computational predictions, of both structures and properties, are in excellent agreement with our experimental results, we show that our high throughput methods are equally useful as tools to rank MOFs from best to worst – significantly reducing time spent on the synthesis of low performance materials.