the ENERGY lab

R&D FACTS

Chemistry & Surface Science

The Rational Design and Synthesis of CO_2 Capture Materials

Background

One quarter of the world's coal reserves is located in the United States. The energy content of these resources exceeds all of the world's known recoverable oil. Coal is also the workhorse of our national electric power industry, responsible for more than half the electricity consumed by Americans. Nonetheless, managing CO_2 emissions from its utilization is perhaps the largest technical and political challenge faced by the fossil energy industry. Although CO_2 is routinely separated and captured as a by-product from industrial processes, existing capture technologies are not necessarily cost-effective for sequestering CO_2 from power plants. To address this challenge, NETL's Office of Research and Development (ORD) has initiated cutting-edge research aimed at developing robust classes of CO_2 capture materials that can easily be optimized for essentially any end-use application. The approach is multi-faceted and combines new advances in the rational synthesis of chemical sorbents with computational methodologies that lead to the rapid discovery, production, and testing of new capture materials.

The Interplay Between Experiment and Computation

Traditional sorbent design typically uses a trial-and-error approach which relies on using "intuition" to produce new materials which are then tested until matched with an application suited for their properties. Recent advances in synthetic chemistry at NETL have created a platform where sorbents can be designed and synthesized in a rational fashion to have specific pore sizes, shapes, or functional groups allowing researchers to produce materials optimized for a specific end use application. This sorbent design platform is based on a series of porous coordination polymers (PCPs), which use small metal clusters in conjunction with organic and inorganic linkers to create a crystalline porous material. Control of the pore's size, shape, and functionality are achieved by a rational choice of linker molecules and metal clusters during the synthetic step. The nearly limitless combination of linkers and metal clusters makes this platform ideal for computational chemistry studies, which can easily screen thousands of combinations and guide experimental researchers to the most promising candidates. These candidates are then produced in the laboratory and tested for capture applications.

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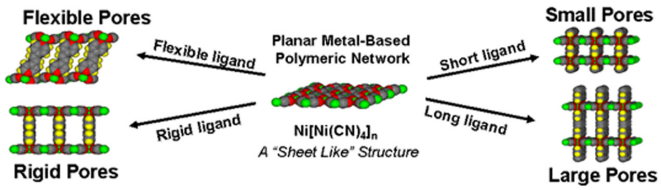
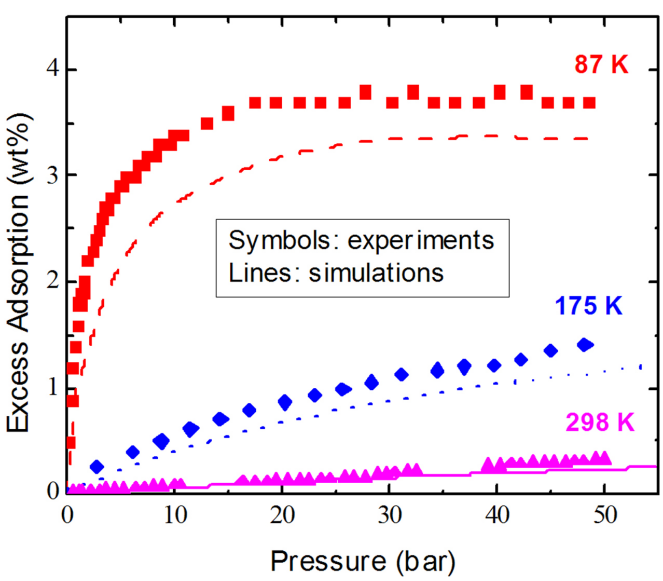


Synthetic scheme illustrating how a simple metal cluster system can be transformed into a porous CO_2 material by using different types of linking ligands. Computational researchers focus on screening different combinations of ligands and metal clusters to predict the most promising systems, which are then synthesized by chemists at NETL.

The interplay of experimentalists and computational scientists relies heavily on the computational team's ability to accurately predict the storage capacity of new materials. At NETL, researchers have focused specifically on developing experimental protocols that provide the input needed to refine the computational models used for this predictive work. These protocols involve combining experimentally determined structural data with thermodynamic information (enthalpies of adsorption) on a series of baseline materials. Once agreement is achieved with these baseline systems, computational researchers can then move forward to rapidly screen new materials and guide synthetic efforts towards the most promising candidates.



A series of adsorption isotherms illustrating how computational researchers are able to predict experimental results for storage materials. The symbols represent experimental data and the lines illustrate the predictions of refined computational models.

Testing Sorbents for Large-Scale Deployment

Once they have been identified, promising sorbents must be further evaluated for the performance and cost issues associated with deployment in power plants and other end-use applications. For this level of analysis, researchers in ORD collaborate with colleagues from NETL's Office of Systems, Analyses and Planning (OSAP). OSAP conducts studies of complex, large systems, such as industrial or ecological processes, and the interactions amongst those systems, including social, economic, political, regulatory, technological, design, and management institutions. For the design of emerging technologies, such as PCP sorbents for CO_2 capture, OSAP researchers use experimental isotherms and other data determined by ORD's staff and simulate the behavior of these sorbents deployed in pre- or post-combustion capture applications. OSAP's analysis can guide sorbent research at NETL by benchmarking the performance of new sorbents against more mature technologies, evaluating the material costs of new sorbents during deployment, and testing any new process conditions that the new sorbents require which may outperform or cost less than standard technologies used in the field. The initial testing conducted by OSAP provides specific targets for ORD's researchers to focus on to improve a sorbent's performance. The flexible synthetic platform developed by ORD chemists for producing these sorbents allows them to make these adjustments to meet the targets defined by OSAP.