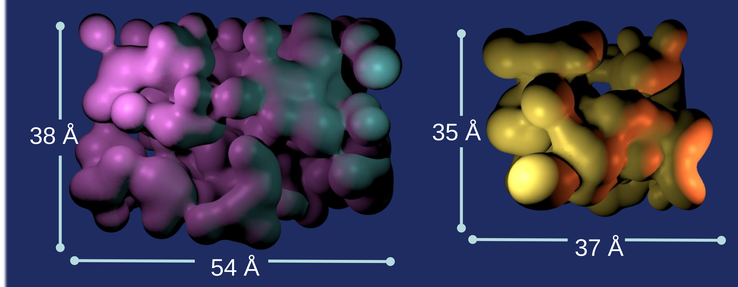
Discovering the Theoretical Limits of Oxygen Storage within Nanoporous Materials

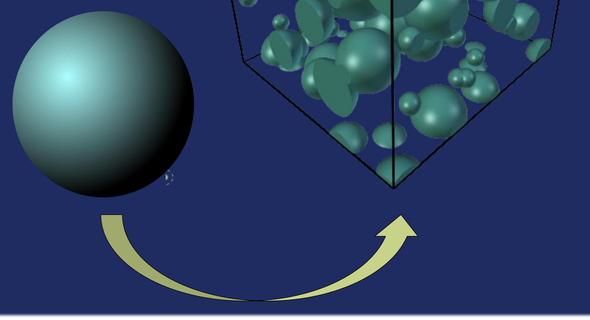
How much oxygen can porous materials store?

Nanoporous materials present an opportunity for improved oxygen storage. Determining a theoretical limit for the maximum amount of oxygen that can be stored in these materials would accelerate the discovery of new materials by providing a narrowed material space for researchers to explore. Our approach uses algorithmic design of hypothetical materials to define a theoretical limit for oxygen storage within nanoporous materials at 298 K and 30 bar.

Algorithmic Design of Hypothetical Materials

10000 hypothetical materials were generated by an algorithm that randomly assigns values, within a range, for potential well-depth (ε), radius of interaction (σ), number density, unit cell dimensions, and partial charge. Lennard Jones (LJ) limits were selected to be 25% lower and higher than values defined in the Universal Force Field (UFF).





$$V_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Parameter	min	max
Unit cell (x,y,z) (Å)	14.81	52.39
σ (Å)	1.89	5.46
ε (m^2kg/s^2)	1.58	427.72
Number Density (atoms/$Å^3$)	0.00848	0.000013
Charge (*e*)	-3	3

Analysis of oxygen adsorption data suggests **a theoretical limit for oxygen storage within porous materials of 600 cc/cc at 30 bar and 298K**. Based on analysis of adsorption data of 10000 hypothetical materials, storage beyond 600 cc/cc appears physically impossible, regardless of the material being used. Analysis of down-selected libraries, with more conservative force-field parameters yields lower theoretical limits, may prove useful as storage targets for various applications. The *20% parameters* library had a maximum oxygen adsorption of 526 cc/cc and the *40% parameters* library had a maximum of 376 cc/cc.

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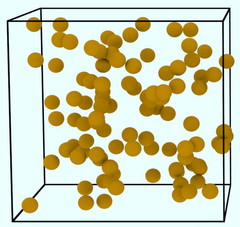
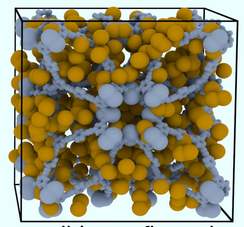
Grand Canonical Monte Carlo (GCMC) simulations were used to screen 10000 randomly generated hypothetical materials for oxygen adsorption, helium void fraction (HVF), and BET surface area at 30 bar and 298 K. The size of the library was reduced from 10000 to 392 by lowering the maximum allowable LJ parameters and partial charges in the framework.

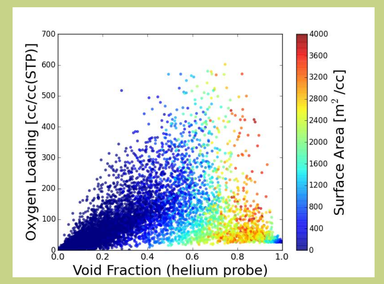
Prediction of oxygen storage using GCMC simulations



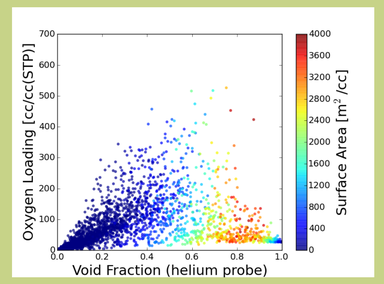
Oxygen reservoir at 30 bar and 298 K



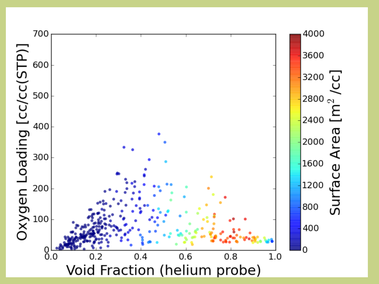
One possible configuration of oxygen in a porous material



10000 materials
100% parameters



2615 materials
20% parameters



392 materials
40% parameters