

Sorption

Producers of industrial and utility gases, petrochemicals, and specialty catalysts gain huge commercial benefits from improving processes dependent upon sorption. Molecular adsorption into microporous structures such as zeolites, aluminophosphates, or polymers is crucial in numerous applications including air separation, hydrocarbon cracking, gas sensors, and ion exchange.

Sorption provides a means of predicting fundamental properties, such as sorption isotherms (or loading curves) and Henry's constants, needed for investigating separations phenomena. In addition, modeling can be used to rationalize sorption properties in terms of molecular level processes. How, for example, do pore size, molecular weight, and density of acid sites affect the ability of a zeolite to separate molecules? Typically, experimental characterization requires synthesis followed by measurement of physical properties. With simulation, lead time to development of optimized systems can be significantly reduced and experimental effort can be guided by rational design.

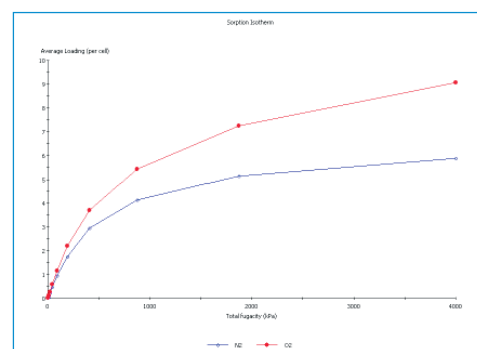
How Sorption Benefits You

Sorption provides a solution for the prediction of molecular adsorption in crystalline materials and on surfaces. An advanced simulation is combined with sophisticated structure modeling tools in the Materials Studio desktop environment enabling you to:

- predict adsorption isotherms;
- model the effects of structural changes, ion exchange, differing charge distributions and substitutional disorder on sorbing properties;
- study the behavior of pure components or mixtures in molecular sieves;
- quantify the effects of temperature and pressure on the system;
- understand the fundamentals of the sorption mechanism at the atomistic level by identifying preferential sorption sites and computing binding energies;
- interpret results through powerful graphical representations and analysis.

Knowledge of these fundamental properties is often essential for describing many industrially relevant problems. For example, adsorption isotherms are necessary for describing the diffusion of molecules through membranes, yet

experimental data are often lacking. Furthermore, the results gained from molecular modeling can provide insight not easy available through experiment. Shape selectivity of zeolites in hydrocracking, for example, can be understood in terms of preferential sorption sites in the pores.



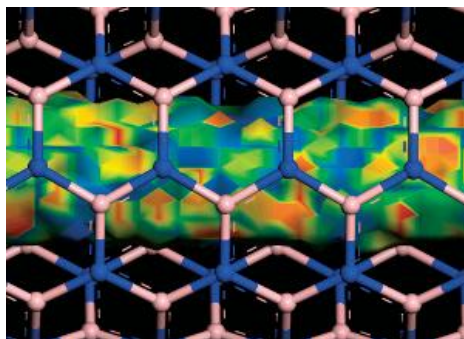
Sorption isotherms for O₂ and N₂ in mordenite at 300 K as computed by Sorption. The ability to handle mixtures of sorbates is critical to modeling processes of separations and diffusion.

What can Sorption do?

Sorption allows you to simulate a pure sorbate (or mixture of sorbate components) absorbed in a sorbent framework, typically a microporous crystal such as a zeolite, or on a surface such as a metal oxide. Sorption provides three ways of simulating the sorption equilibrium

Materials Studio Datasheet

- Fixed loading (canonical ensemble): determine the preferred binding sites & energies for a fixed number of sorbates
- Fixed pressure (grand canonical ensemble): predict the amount of sorbate at a given temperature and pressure
- Henry constant (uniform ensemble): compute the limit of sorbate loading as pressure approaches zero.



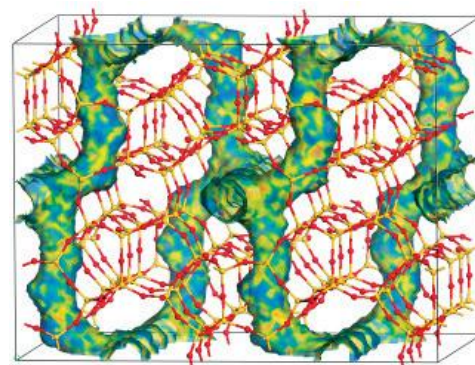
Sorption can be used to study gas storage in nanotubes. The figure represents H₂ sorption in a boron-nitride nanotube. Nitrogen atoms are blue and Boron pink. The surface illustrates an isodensity surface of H₂ mass density within the nanotube. The surface is colored by the potential energy: red indicates lower energy (tighter binding) and blue higher energy.

Sorption supports two Monte Carlo simulation methods: the Metropolis Monte Carlo method and the Configurational bias Monte Carlo method. The Metropolis method is a conventional Monte Carlo method in which the sorbate structure is treated as rigid, and only rigid body translations and reorientations are incorporated. The Configurational bias method additionally includes torsional degrees of freedom. The Configurational bias method is useful for large flexible sorbates, for which the Metropolis method becomes inefficient.

The Materials Studio Advantage

Sorption is a Materials Studio® product. Materials Studio provides a user-friendly interface, complying with Windows® standards. Materials Visualizer, the core Materials Studio product, offers a wide range of model building and visualization tools that allow you to rapidly construct models of the systems of interest, select Sorption with two mouse clicks, and run a Monte-Carlo simulation.

A flexible client-server architecture means that calculations can be run on Windows XP, Linux, running on Intel 32 bit compatible systems, and IRIX servers located elsewhere on your network. Results are returned to your PC, where they may be displayed and analyzed. You can easily produce high quality graphics of mass density and potentials. Structures, graphs, and images can be instantly exchanged with other PC applications, facilitating exchanging data with colleagues, writing reports, or manipulating the Sorption output with spreadsheets or other applications.



Representation of the sorption of CH₄ in zeolite MFI at 100 kPa and 300°K. The figure shows an isodensity surface of the predicted locations of CH₄, colored coded by the binding energy. Lower energy (more tightly bound) areas are in red and high energy areas are blue. A representation of this type will indicate areas of highest concentration of the sorbates as well as preferred binding sites in the cavities.