BIOVIA MATERIALS STUDIO ADSORPTION LOCATOR

DATASHEET

Understanding adsorption phenomena is of key importance in coatings development and also in catalysis, gas sensors, and general materials discovery. Deposition processes, storage devices, corrosion problems, and catalysis on microporous materials are examples of processes that can benefit from a better understanding of adsorption phenomena.

BIOVIA Materials Studio Adsorption Locator helps you find the most stable adsorption sites for a broad range of materials, including zeolites, carbon nanotubes, silica gel, and activated carbon—to name just a few. This information can help you gain further insight about your system, such as the most likely point of attack for corrosion on a surface, the most stable site for atomic layer deposition, the most effective zeolite for a particular synthesis, and the likelihood of nanotube activation by a particular adsorbate. With such knowledge at hand, you will be able to better guide subsequent screening experiments, saving both time and money.

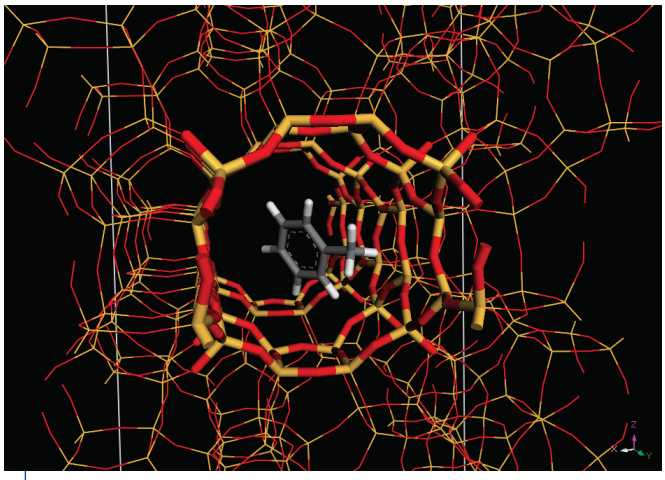

Figure 1: BIOVIA Materials Studio Adsorption Locator can be used to find the most stable adsorption sites for a broad range of materials. The image shown here illustrates the most stable configuration of toluene adsorbed in a BEAzeolite pore.

BETTER UNDERSTAND SURFACE PHENOMENA

BIOVIA Materials Studio Adsorption Locator allows you to simulate a substrate loaded with an adsorbate or an adsorbate mixture, as shown in Figure 1. Adsorbates can be molecular gases or liquids. The application is designed to find low energy adsorption sites for both periodic and nonperiodic ubstrates. By using BIOVIA Materials Studio Adsorption Locator in conjunction with other sophisticated tools in the BIOVIA Materials Studio modeling and simulation environment, you can:

- predict the most stable adsorption site for a broad range of materials
- screen thousands of conformations to find the most stable one
- find active sites on a nanocatalyst
- locate the most stable positions on a surface for atomic layer deposition processes
- study how different molecules interact with molecular sieves (e.g. zeolites)
- dock multiple additives onto a substrate
- understand the adsorption process at the atomistic level (structure influence, additive effects)
- predict adsorption energies

The fundamental knowledge gained from BIOVIA Materials Studio Adsorption Locator simulations provides a better understanding of important surface phenomena—something that cannot be easily inferred from experiment alone. For example, the atomistic and molecular interactions examined are key aspects to understanding bonding at interfaces, which is important in atomic/molecular deposition as well as in coatings development. Shape-selective catalysis can benefit from BIOVIA Materials Studio Adsorption Locator screening studies on zeolites, while studies of carbon nanotubes can be helpful in the design of sensors and storage devices.

HOW IT WORKS

BIOVIA Materials Studio Adsorption Locator identifies possible adsorption configurations by carrying out Monte Carlo searches of the configurational space of the substrate-adsorbate system as the temperature is slowly decreased (simulated annealing). This process is repeated to identify additional local energy minima. Adsorbates are typically molecular gases or liquids, and substrates are usually solid surfaces (crystalline or amorphous), porous materials, or large molecules (e.g. carbon nanotubes, nanocatalysts). You can select a force field, specify the accuracy level, and choose methods for calculating charges and non-bond interactions.

	A	B	C	D	E	F
	Structures	Total energy	Adsorption energy	Rigid adsorption energy	Deformation energy	toluene : dEad/dNi
1	Substrate	0.00000000				
2	toluene	82.55018241				
3	BEA - 1	-15.81677590	-98.36695831	-27.51929474	-70.84766357	-98.36695831
4	BEA - 2	-15.60161110	-98.15179350	-27.29258133	-70.85921217	-98.15179350
5	BEA - 3	-15.26063823	-97.81082064	-26.93141378	-70.87940686	-97.81082064
6	BEA - 4	-15.01063892	-97.56082133	-26.72404399	-70.83677734	-97.56082133
7	BEA - 5	-14.67703353	-97.22721594	-26.35127583	-70.87594011	-97.22721594
8	BEA - 6	-14.42141784	-96.97160024	-26.08479261	-70.88680763	-96.97160024
9	BEA - 7	-14.19731023	-96.74749263	-25.88994915	-70.85754348	-96.74749263
10	BEA - 8	-13.89172589	-96.44190829	-25.56335872	-70.87854957	-96.44190829
11	BEA - 9	-13.54609430	-96.09627671	-25.21321255	-70.88306416	-96.09627671
12	BEA - 10	-13.31998746	-95.87016987	-25.01596859	-70.85420128	-95.87016987
13	BEA - 11	-13.07749100	-95.62767340	-24.74501231	-70.88266109	-95.62767340
14	BEA - 12	-12.22314472	-94.77332713	-23.91491703	-70.85841010	-94.77332713
15	BEA - 13	-11.77655717	-94.32673957	-23.46643270	-70.86030687	-94.32673957
16	BEA - 14	-11.51786627	-94.06804868	-23.17492568	-70.89312300	-94.06804868

Figure 2: This study table obtained from an BIOVIA Materials Studio Adsorption Locator calculation displays the most stable substrate-adsorbate configurations for several energy ranges, illustrating how easy it is to model and compare many configurations.

BIOVIA Materials Studio Adsorption Locator gives you tremendous flexibility in defining the region of the substrate that you want to explore. This allows you to focus on the most chemically-significant regions of your system. Several different approaches are possible through the graphical user interface, including:

- **Bounding box:** define a volume surrounding the entire substrate within which the adsorbate components can be added
- **Set of atoms:** specify a group of atoms in the substrate structure and restrict the search to a region around them
- **3D field values:** define the search region by the volume of field, such as one defined by a solvent accessible surface; the adsorption volume can be adjusted by changing the display range of the field

After running your simulation, BIOVIA Materials Studio Adsorption Locator will output a study table with a specified number of low energy configurations, as shown in Figure 2. You can choose to compute the most stable substrate-adsorbate configurations; or you can receive representative configurations from a broader range of the configurational space that is being explored.

INTEGRATE YOUR MODELING AND SIMULATION WORKFLOWS

As part of the BIOVIA Materials Studio modeling and simulation environment, BIOVIA Materials Studio Adsorption Locator benefits from integration with several advanced building and visualization tools. For example, nanobuilders in BIOVIA Materials Studio Visualizer make it easy to build and bundle together carbon nanotubes, as well as nanoclusters of different shapes. Those structures can then be used as substrates in BIOVIA Materials Studio Adsorption Locator, as shown in Figure 3.

Similarly, initial screening results from BIOVIA Materials Studio Adsorption Locator can easily be input into an automated search and optimization workflow. For example, you could use the configurations obtained from an BIOVIA Materials Studio Adsorption Locator calculation as input for a BIOVIA Materials Studio DMol^3 quantum mechanics-based calculation in order to obtain more accurate adsorption energies. You could then perform a BIOVIA Materials Studio QSAR statistical analysis of the results for all the substrates studied, helping you quickly screen all potential substrates that could be used in the design of a particular coating, sensor device or catalysis route.

To learn more about BIOVIA Materials Studio, go to **accelrys.com/materials-studio**

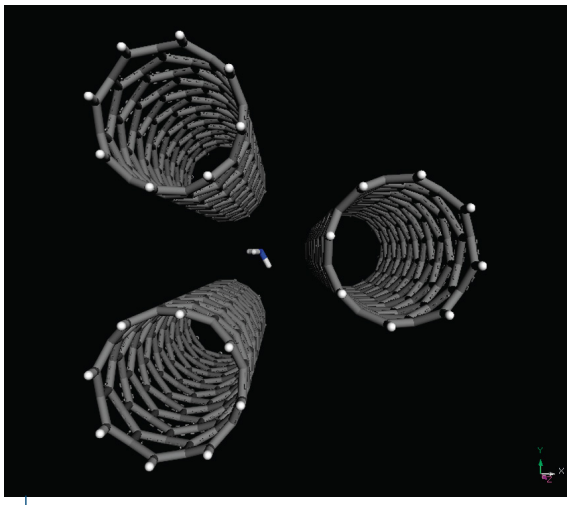

Figure 3: Advanced building and visualization tools in BIOVIA Materials Studio Visualizer can be used to create structures to use as substrates in BIOVIA Materials Studio Adsorption Locator. Here, an ammonia molecule is absorbed in the groove between three carbon nanotubes.

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