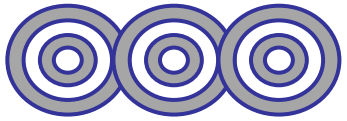
CHEM 652
Applied Analytical Chemistry



Materials Studio - An Overview

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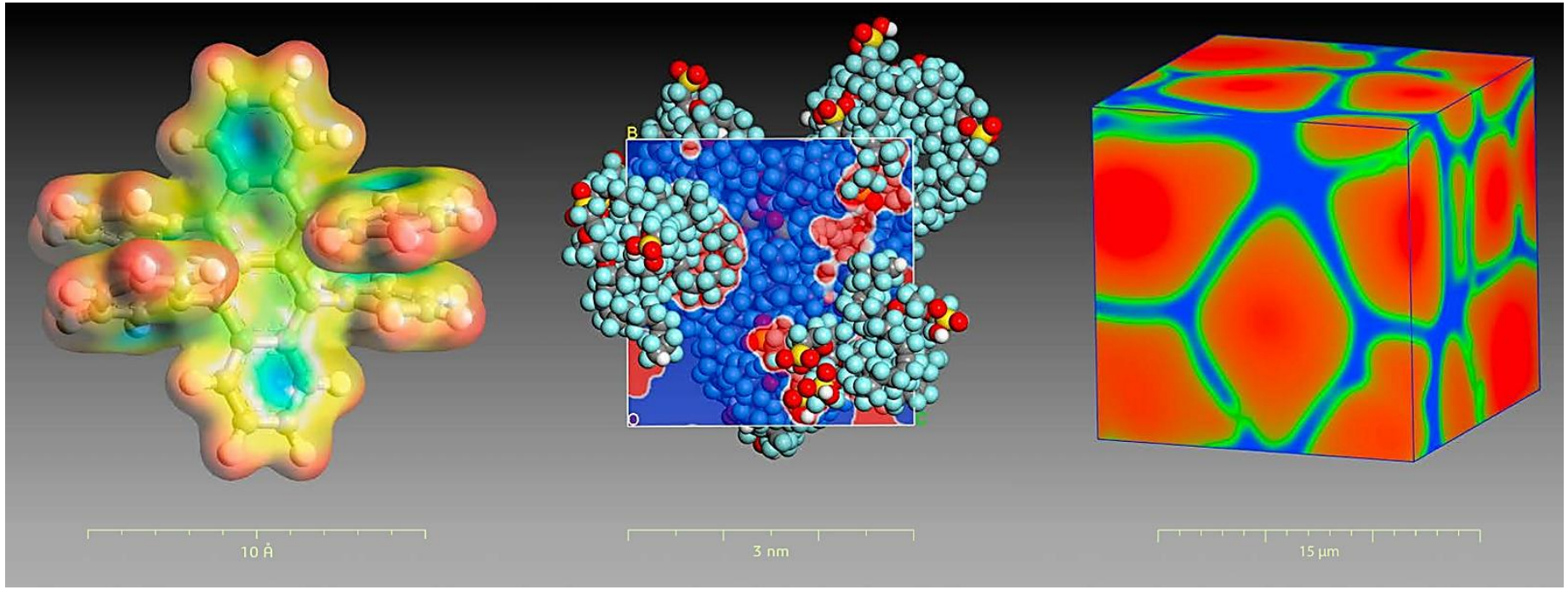
Advanced Materials Research Chair
AMRC

جامعة الملك سعود
King Saud University

MATERIALS STUDIO

Materials Studio



DASSAULT SYSTEMES

accelrys®

Materials Studio® is a complete modeling and simulation environment (software) that enables researchers in materials science and chemistry to develop new materials by predicting the relationships of a material's atomic and molecular structure with its properties and behavior.

Materials Studio is developed and distributed by BIOVIA (formerly Accelrys).

Using Materials Studio, researchers in many industries can engineer better performing materials of all types, including;

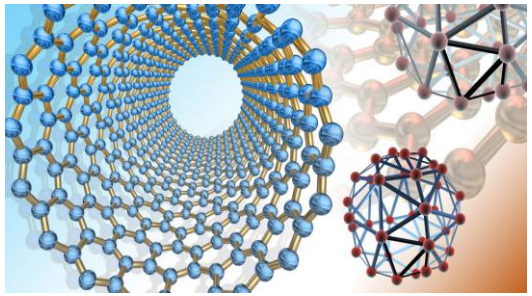
Chemicals & Catalysts

Pharmaceutical Development

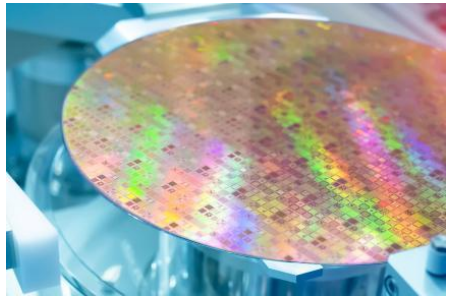
Polymers & Composites

Metals & Alloys

Nanomaterials



Semiconductors



Consumer Packaged Goods

Batteries & Fuel Cells

Electronics

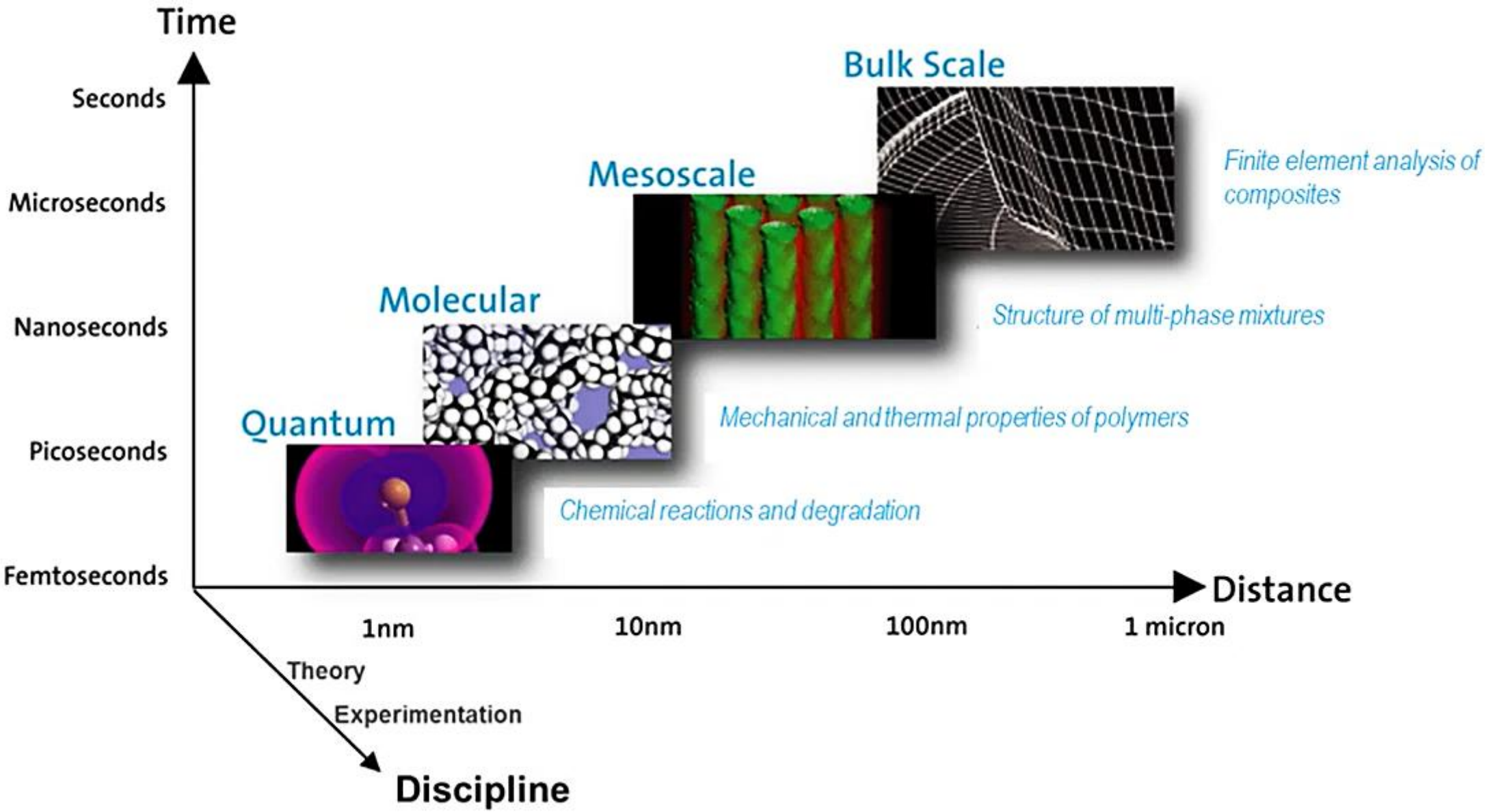
VISUALIZATION

Chemists, polymer scientists, and other materials scientists become productive faster and with less effort using Materials Visualizer, the easiest to use and most complete graphical user environment for materials modeling and simulation.

Materials Studio Visualizer provides capability to construct, manipulate and view models of molecules, crystalline materials, surfaces, polymers, and mesoscale structures. It also supports the full range of Materials Studio simulations with capabilities to visualize results through images, animations, graphs, charts, tables, and textual data.

SOLUTION TECHNOLOGIES

Materials Studio provides a complete range of simulation capabilities from quantum, atomistic, mesoscale, statistical, analytical and crystallization tools. Its' broad range of solutions enable researchers to evaluate materials at various particle sizes and time scales in order to predict properties more accurately and evaluate performance in the shortest time possible.


Time
Seconds
Microseconds
Nanoseconds
Picoseconds
Femtoseconds
Bulk Scale
Mesoscale
Molecular
Quantum
Finite element analysis of composites
Structure of multi-phase mixtures
Mechanical and thermal properties of polymers
Chemical reactions and degradation
Distance
1nm
10nm
100nm
1 micron
Theory
Experimentation
Discipline

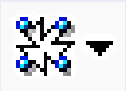
QUANTUM TOOLS

Materials Studio provides a range of quantum mechanics-based tools for molecules and periodic structures, including density functional methods, linear scaling DFT, QM/MM and semi-empirical tools. These tools provide accurate results for the structural, thermophysical, electronic, and optical properties of materials.

Product	Icon	Description
CASTEP		Simulates the properties of solids, interfaces, & surfaces for a wide range of materials including ceramics, semiconductors, & metals using a plane-wave density functional method.
DMol^3		Is used to model the electronic structure and properties of organic and inorganic molecules, molecular crystals, covalent solids, metallic solids, & infinite surfaces using DFT.
DFTB$^+$		Is a semi-empirical module for simulating electronic properties of materials. It uses a tight-binding approach based on density functional theory to enable quantum mechanical accuracy on larger system sizes.
VAMP		Is capable of rapidly predicting many physical & chemical properties for molecular systems using a semi-empirical molecular orbital method. It is an ideal intermediate approach between forcefield & first principles methods.
ONETEP		Is a linear scaling DFT code, enabling accurate, first principles calculations on systems of up to thousands of atoms.
QMERA		Employs QM/MM method combining the accuracy of a quantum with the speed of a forcefield calculation. This approach makes it possible to perform accurate calculations on very large systems for substantially less effort.
CANTERA		Is a solver for chemical rate equations. Cantera provides environment for configuring the thermodynamic input, and for executing these calculations. Cantera Reaction Editor enables users to introduce new species and reactions, optionally with reaction rates determined from Materials Studio DMol^3, into complex reaction schemes with existing experimentally determined thermodynamic data.
KINETIX		Is a program for simulating the competing chemical and physical adsorption, desorption and diffusion processes taking place at surfaces. This provides unique insights such as the role of species diffusion in catalyst activity and poisoning, and surface coverage of species at up to microscales.
FlexTS		Is a robust tool for identifying the minimum energy path between reactant and products in chemical reactions (location of transition states). FlexTS requires DMol3 or DFTB+ in order to supply the system energy of each configuration.
NMR CASTEP		Predicts NMR chemical shifts and electric field gradient tensors from first principles. The method can be applied to compute the NMR shifts of both molecules and solids for a wide range of materials including ceramics and semiconductors.

CLASSICAL SIMULATION TOOLS

Materials Studio offers a very wide range of methods based on classical interactions between atoms and molecules. These include Molecular Dynamics, Lattice Dynamics and various Monte Carlo based methods as well as the provision of forcefields.

Product	Icon	Description
Adsorption Locator		Finds low-energy adsorption sites for molecules on both periodic & non-periodic substrates.
Sorption		Provides a means of predicting fundamental properties needed for investigating adsorption & separations phenomena, such as sorption isotherms & Henry's constants.
Amorphous Cell		Is a suite of computational tools that allow you to construct representative models of complex amorphous systems & to predict key properties.
Blends		Predicts phase diagrams and interaction parameters for liquid-liquid, polymer-polymer, and polymer-additive mixtures, phase equilibria, & separations technology.
Conformers		Provides conformational search algorithms & analysis tools to characterize molecular conformation & flexibility.
Forcite Plus		Offers molecular mechanics and dynamics methods for molecules & periodic systems. The tool includes a wide range of analysis features to predict mechanical properties, diffusivity, local structure, density variations, cohesive energy density, dipole autocorrelation functional & more.
GULP		Is a method for optimization, property calculation & dynamics of materials. It includes a wide range of forcefields for metals, oxides, minerals semiconductors, as well as molecular mechanics forcefields for covalent systems. Forcefield fitting tools are also provided to develop parameters for custom materials.
COMPASS		Is a forcefield which enables accurate prediction of structural, conformational, vibrational, & thermophysical properties for a broad range of molecules in isolation & in condensed phases, and under a wide range of conditions of temperature & pressure.

MESOSCALE SIMULATION TOOLS

Mesoscale methods in Materials Studio are based on a coarse-graining approach, whereby groups of atoms are replaced by beads. These methods enable the modeling of behavior at length and time scales which are beyond the range of classical tools.

Product	Icon	Description
MesoDyn		Is a classical density functional method for studying the long length- and time-scale behavior of complex fluid systems, in particular the phase separation and structure of complex polymer systems.
Mesocite		Is a coarse-grained simulation module for the study of materials at length scales ranging from nanometers to micrometers and time scales from nanoseconds to microseconds. Mesocite can provide structural and dynamic properties of fluids in equilibrium, under shear or in confined geometries.
PhaseField		Is a module providing predictions of microstructure in hard materials such as grain structure in complex metal alloys through simulation of solidification and grain growth. This module is run using protocols provided by Pipeline Pilot Materials Studio Collection.

STATISTICAL TOOLS

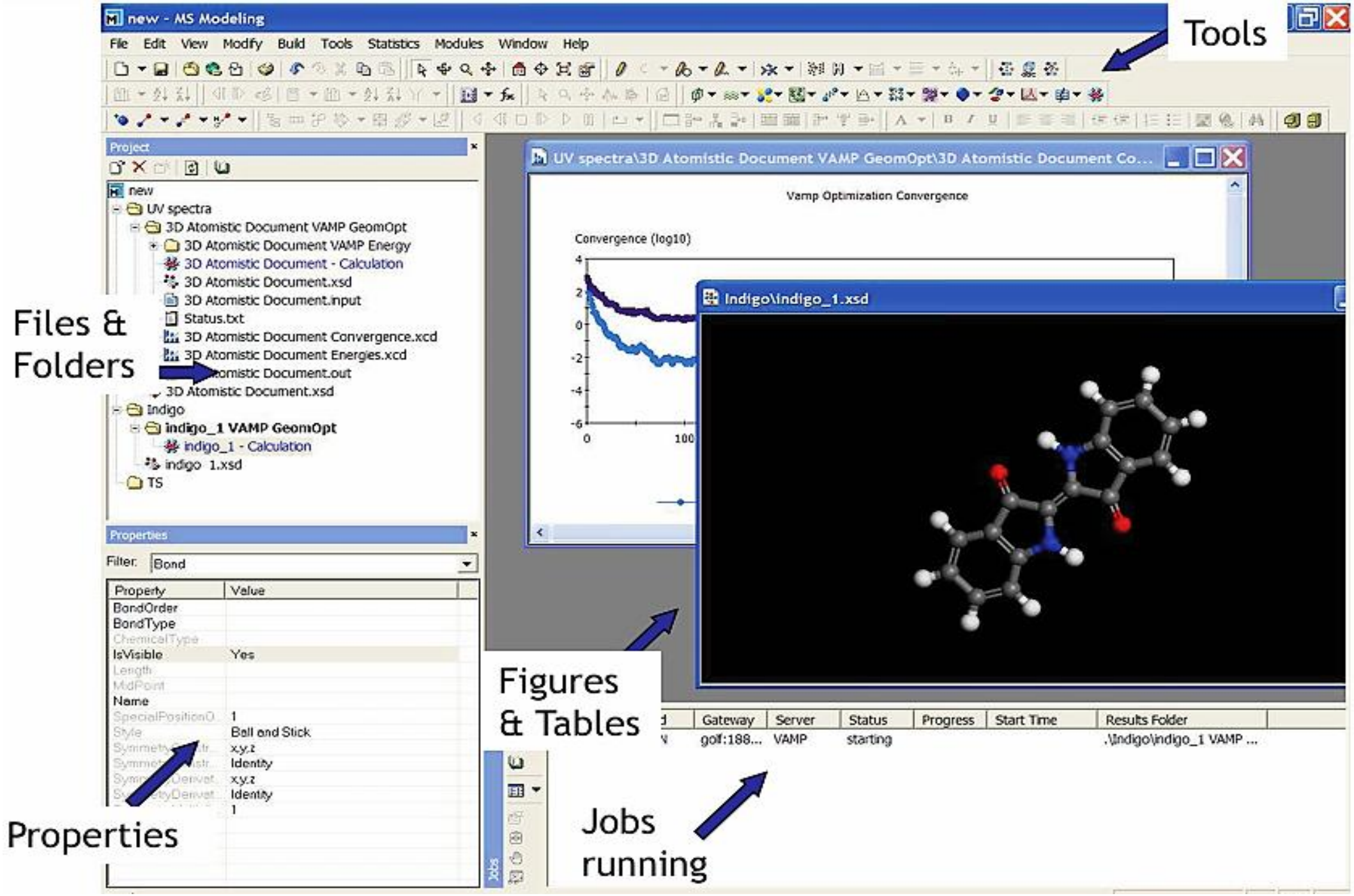
Statistical tools are ideal to screen compounds quickly by relating molecular traits directly to experimentally observed quantities.

Product	Icon	Description
QSAR		QSAR's (Quantitative Structure-Activity Relationships) integration in Materials Studio provides access to a wide range of descriptors and advanced analysis capabilities to help generate high quality structure activity relationships. QSAR includes a wide range of descriptors including topological and electro-topological descriptors. Also, Jurs descriptors enable charge distribution on solvent surfaces to be examined; VAMP Descriptors further extend the range of 3D descriptors into those including electronic interactions; and GFA applies a sophisticated genetic algorithm method to calculate quantitative structure-activity relationships.
QSAR Plus		Adds the power of the DMol3 Descriptors for calculating reactivity indices and accurate energies to QSAR. Also included are Neural Networks to build non-linear models and models that are more resistant to noisy datasets than other model building methods. It can also be used with datasets that have some missing values, and can be used to build weighted models to predict multiple physical properties.
Synthia		Calculates properties of homo- and copoplymers using advanced Quantitative Structure-Property Relationships (QSPRs). It allows researchers to rapidly screen candidate polymers for a wide range of properties.

ANALYTICAL & CRYSTALLIZATION TOOLS

Analytical and crystallization tools are employed to investigate, predict, and modify crystal structure and crystal growth.

Product	Icon	Description
Morphology		Allows you to predict crystal morphology from the atomic structure of a crystal. Morphology allows for the prediction of crystal shape, the analysis of crystal surface stability, the development of tailor-made additives, & the control of solvent & impurity effects.
Polymorph		Predictor has been developed for use with fairly rigid, non-ionic or ionic molecules composed primarily of carbon, nitrogen, oxygen, & hydrogen. The approach is based on the generation of possible packing arrangements in all reasonable space groups to search for the low-lying minima in lattice energy.
Polymorph Predictor		Allows you to predict potential polymorphs of a given compound directly from the molecular structure.
Motif		Analyzes connectivity information in molecular crystals, providing a qualitative & quantitative analysis method of hydrogen bond topologies. Combined with the predictive capabilities of Materials Studio Polymorph, Motif allows for categorization & statistical scoring of proposed structures. It interfaces with the Cambridge Structural Database exploiting Cambridge Crystallographic Data Centre's Mercury functionality.
Reflex		Simulates X-ray, neutron, & electron powder diffraction patterns based on models of crystalline materials. Reflex Plus offers a complete package for the determination of crystal structures from medium- to high-quality powder diffraction data.
Reflex QPA		Extends the Reflex functionality for quantitative phase analysis, allowing for the determination of the relative proportion of different phases, including both inorganic as well as organic systems, in a mixture based on powder diffraction data.
X-Cell		Is an efficient, indexing algorithm for medium- to high-quality powder diffraction data. X-Cell uses an extinction-specific dichotomy procedure to perform an exhaustive search of parameter space to establish a complete list of all possible unit cell solutions.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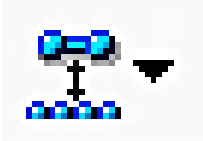
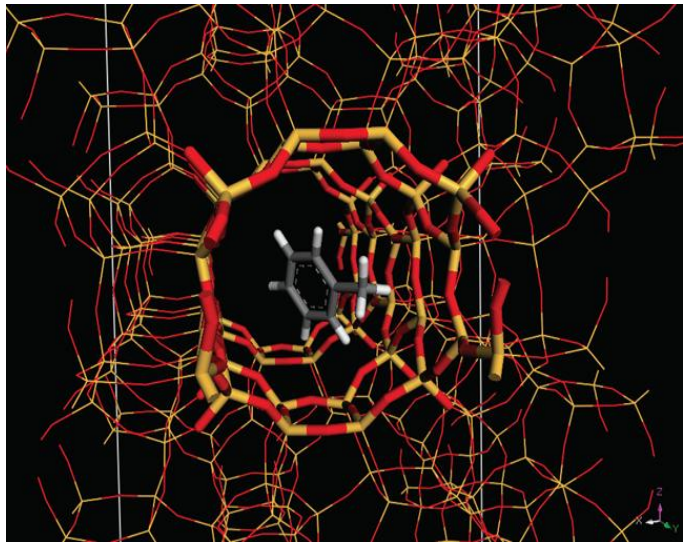
Adsorption Locator

A tool that allows you to find low energy adsorption sites on both periodic and nonperiodic substrates. This tool determines energetically favourable positions of an adsorbate in periodic and aperiodic structures.

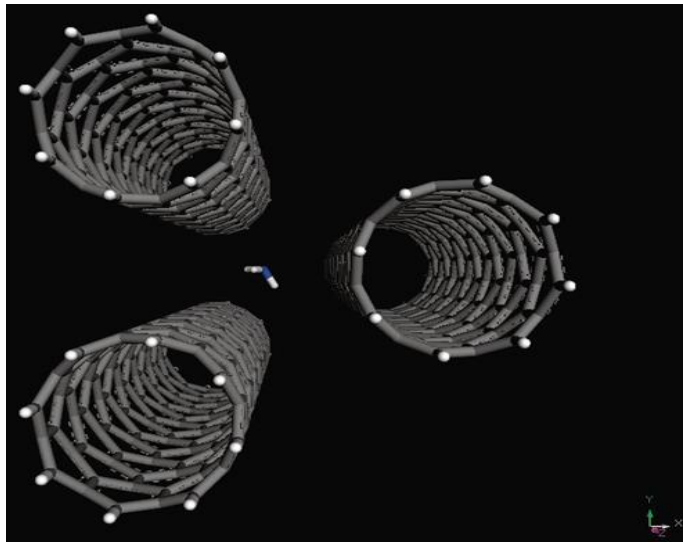




Adsorption Locator can be used to find the most stable adsorption sites for a broad range of materials

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

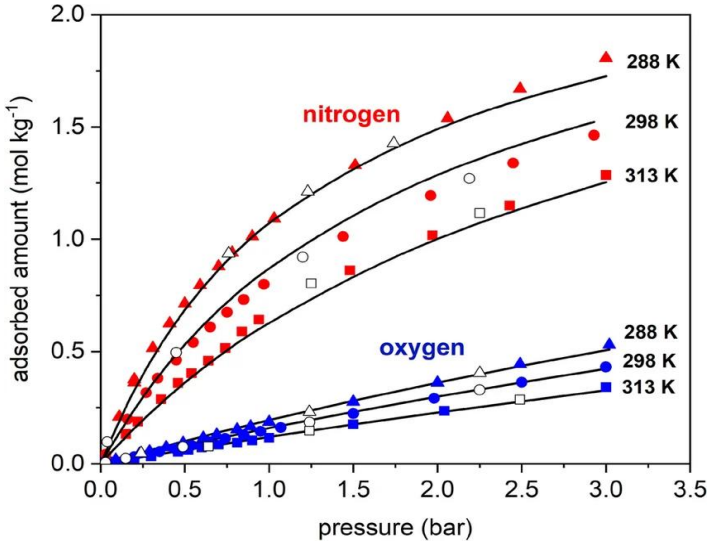
	A	B	C	D	E	F
	Structures	Total energy	Adsorption energy	Rigid adsorption energy	Deformation energy	toluene : dEad/dNi
1	Substrate	0.00000000				
2	toluene	82.55018241				
3	BEA - 1	-15.81677590	-98.36695831	-27.51929474	-70.84766357	-98.36695831
4	BEA - 2	-15.60161110	-98.15179350	-27.29258133	-70.85921217	-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



Adsorption Locator can be used to create structures to use as substrates in BIOVIA Materials Studio Adsorption Locator

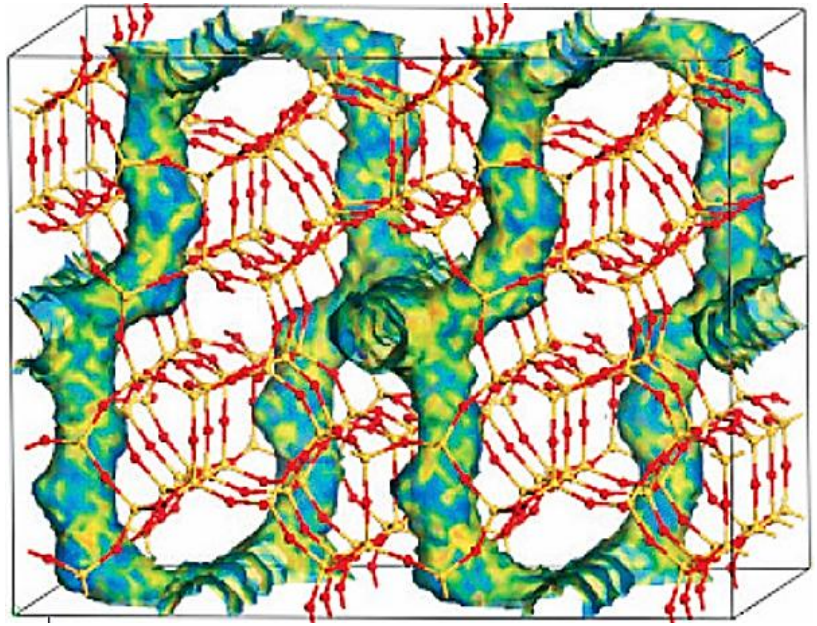
Sorption

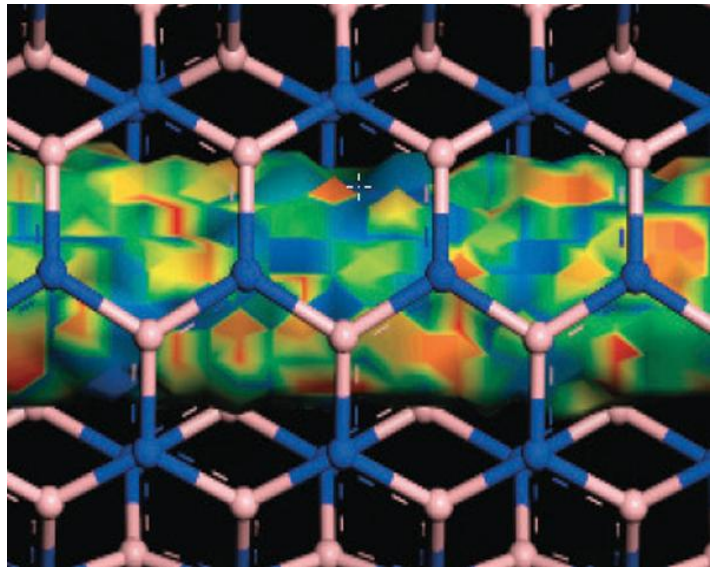
A tool that allows you to simulate a sorbate absorbed in a sorbent framework in order to calculate properties such as adsorption isotherms, binding sites and energies, density and energy fields, energy distributions, isosteric heats, and Henry constants.



Sorption isotherms for O_2 and N_2 in mordenite at different temperatures as computed by Materials Studio Sorption. The ability to handle mixtures of sorbates is critical to modeling processes of separations and diffusion

Sorption of CH_4 in zeolite at 100 kPa and 300K. The figure shows an isodensity surface of the predicted locations of CH_4 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





Sorption can be used to study gas storage in nanotubes. The figure represents H_2 sorption in a boron-nitride nanotube. Nitrogen atoms are blue and Boron pink. The surface illustrates an isodensity surface of H_2 mass density within the nanotube. The surface is colored by the potential energy: red indicates lower energy (tighter binding) and blue higher energy


Thank You!