

Exceptional graphics capabilities

Modeling, analysis, and visualization tools for the chemicals and materials based industries

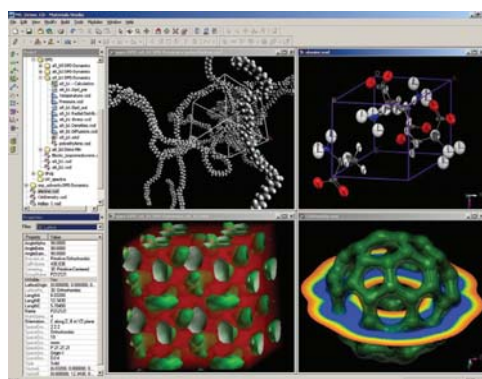
Increase your understanding of materials and improve your communication of chemical information and concepts

Materials Visualizer

Materials Visualizer provides all of the tools that are required to construct graphical models of molecules, crystalline materials, and polymers. You can manipulate, view, and analyze these models. Materials Visualizer also handles graph, tabular, and textual data and provides the software infrastructure and analysis tools to support the full range of Materials Studio® products.

Materials Visualizer is the core product of the Materials Studio software suite, which is designed to support the materials modeling needs of the chemicals and materials-based industries. Materials Studio brings science validated by leading laboratories around the world to your desktop PC.

Materials Visualizer contains the essential modeling functionality required to support computational materials science. It can help you understand properties or processes related to molecules and materials. Materials Visualizer allows you to see models of the system you are studying on your Windows desktop, increasing your understanding by allowing you to visualize, manipulate, and analyze the models. You can also make better use of access to structural data, improve your presentation of chemical information, and communicate problems and solutions to your colleagues very easily.



This is a screenshot of Materials Visualizer, the core Materials Studio product. Materials Studio can display a wide range of materials from bulk amorphous polymers to organic and inorganic crystals. The modules in the Materials Studio suite allow access to tools covering size scales from the quantum to the mesoscale, allowing the calculation of many properties.

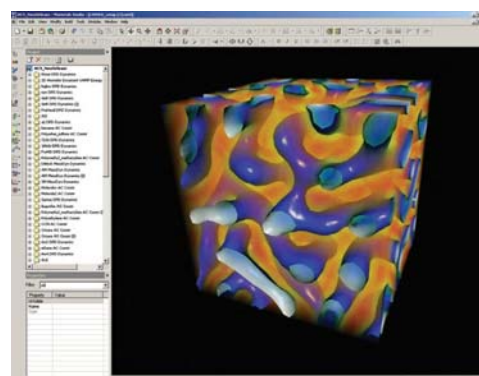


Image of early-stage phase segregation in a diblock copolymer melt. The blue surface indicates the interface between the two components. The volume is colormapped by the density of one of the blocks, red being high density, blue being low-density. The MesoDyn module is used to study these large systems over long-times such as required to observe these structural rearrangements.

What Can Materials Visualizer Do?

Materials Visualizer provides modeling, analysis, and visualization tools, combined with its clear and intuitive graphical user interface. It offers a high-quality environment into which you can plug any Materials Studio product. Within this versatile and completely comprehensive modeling and visualization system, you can:

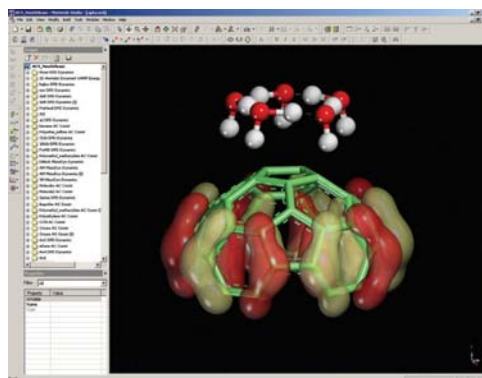
- increase your understanding of materials
- improve your communication of chemical information
- visualize and model structures from chemical databases
- build your own molecules and materials with fast, interactive sketching, building and editing tools
- calculate and display key structural parameters
- display the results of calculations – animated dynamics trajectories, graph data, and molecular models
- use scripting to harvest the full power of Materials Visualizer
- annotate models for pictures and diagrams and produce exceptionally high quality hard-copy output

Materials Visualizer can run on any PC on your network, allowing scientists to use it when and where they need it. Whether used to run a range of Materials Studio modules or as a stand-alone modeling system, Materials Visualizer focuses computational and graphics power on the solution of scientific problems.

Features

Graphical User Interface

- Easy-to-use user interface conforming to Microsoft® standards



Arrangement of water molecules at the tip of a carbon nanotube (CNT). Also displayed is the HOMO, which is seen to be localized on the CNT. Such quantum mechanical calculations have been used to gain insight into the observed influence of water content on conductance in a single-walled CNT.

- Comprehensive, context-sensitive, and fully searchable on-line help, including tutorials covering the main functionality
- Multiple undo/redo
- Project Explorer offers fast, structured access to project data in a standard file explorer view
- Tool and menu bar access to other Materials Studio products
- Tools to manage and monitor calculations on remote or local servers support use of Materials Visualizer with other Materials Studio products
- Management of the default project settings

Display and Communication

- Display, manipulation, and overlay of high quality 3-D graphical models of materials and molecular structure (details follow)
- Display and manipulation of results as 1-D and 2-D graph

data

- Display of model and results data in textual and tabular formats
- Cut-copy-paste to other PC applications for structural, graphical, tabular, and textual data
- File communication with in-house and commercial structure databases
- Supports a wide range of industry-standard file formats for structural, graphical, textual, and experimental data:
 - Structure files: xsd (native), xtd (native), xod (native), msi, car/mdf, cif, mol, sdf, sd,mdl, skc, arc/mdf, his/mdf, acx, trj/msi, .res/.ins (Shelx), pdb, xyz
 - Chart files: xcd (native), csv, tbl
 - Table/ Grid files: xgd (native) csv, tbl, std (native)
 - Text files: txt, htm, pl

Building and Editing Molecular Models

- Fast creation of molecular models using a unique 3-D sketcher
- Automatic hydrogen addition tool for quick molecular sketching
- Fragment sketcher allows fast creation of complex molecules, such as organometallic compounds; includes comprehensive fragment library and tools to enable user-defined fragments
- Clean utility determines good molecular geometries
- Easy editing and input of coordinates and atom properties
- Precise atom/object movement and rotation tools
- Precise atom positioning tools
- User-definition and editing of bond order and hybridization
- Display and editing of the properties of all elements, including a periodic table viewer
- Simple cut, copy, and paste of models and parts of models
- Versatile bond calculation tools
- Symmetry finder for non-periodic systems
- Includes extensive library of molecular, crystalline, and amorphous structures
- Align molecules in specific directions

Specialist Polymer Building Tools

- Polymer builder enables construction of homopolymers, block, and random copolymers, or dendrimers
- Comprehensive library of repeat units
- Tools to enable user-defined repeat units
- Branch generation tool

Specialist Crystal, Surface, and Layer Building Tools

- Crystal builder enables construction of periodic systems based on lattice parameters, atom positions, and symmetry
- Input and editing of symmetry information, including comprehensive space-group information

- Symmetry finder analyzes periodic models and returns symmetry details
- Easy to use supercell creation tool
- Versatile surface builder enables easy surface construction from non-periodic structures using plane group symmetry, or crystals using a cleave method
- Surface builder can create surfaces with vacuum slabs from crystal structures
- Layer builder creates layered structures from either crystalline or amorphous materials, or combinations of both

Analog Building Tools

- Markush library enumeration
- Maintains 3-D geometry
- Specify multiple cores
- R-Groups defined from fragment library

Nanotechnology Building Tools

- Tools available for both single and multi-walled nanotubes
- Specify carbon or boron Nitride tubes
- Build nanoropes
- Create nanoclusters from crystals

Template Building Tools for Mesoscale Structures

- Build templates that can be filled with beads to specify starting conditions for mesoscale calculations
- Add variety of formers such as droplets, rods, slabs, shells, and tubes
- Define size, orientation, position, and priority of formers
- Assign different material fillers to the formers
- Build ordered structures such as micelles and bilayers

Mesoscale Molecule Building Tools

- Powerful tool for building bead representations of molecules
- build simple linear chains and complex branched structures such as dendrimers
- Builds randomized bead structures

General Visualization Tools

- Wide range of display styles—line, stick, ball and stick, space filling spheres (CPK), polyhedral
- Real-time mouse rotation and scaling of models
- Option of orthogonal or perspective views of models
- Full customization of the colors of objects in the model and of the background color
- Choice of a wide range of background textures and images, and the ability to add user-created bitmaps as background images
- Control over rendering quality, including speed-up of model manipulation by 'fast render on move'
- Control over the number of unit cells displayed for a periodic model (including non-integer ranges)
- Display of thermal ellipsoids

- High quality, flexible display of volumetric data from quantum and other calculations (of charge density, potentials, orbitals)
- Display of surface data from quantum and other calculations (of charge density, potentials, orbitals)
- Display of crystal habits including coloring and transparency from morphology calculations
- Control over lighting of the model, including multiple light sources and the ability to alter color and position
- Optional display and labeling of axis and 3-D or 2-D lattices
- Custom coloring of all objects

Model Measurement and Analysis

- Measurement and display of distances, angles, and torsions – updated during structure manipulation
- Create and visualize geometry objects such as principal moments, centres of mass, and planes
- Calculation and display of close contacts and hydrogen bonds
- Calculation and display of solvent and conolly surfaces; includes occupied and accessible volumes and surface areas
- Visualization of Miller Planes for crystals and surfaces
- Superpose multiple physical systems and fit them to either a target or consensus structure using RMS atoms, moment, or field fitting
- Context-sensitive properties explorer provides text display of the properties of atoms and other objects
- Animation of trajectory files (for example, from molecular dynamics)
- Reaction preview and atom matching tools for use as input to transition state searches
- Vibrational analysis tool for displaying and animating normal modes and spectra
- Labeling of molecular models

Field Visualization and Analysis

- Visualize fields as dots or volumes
- Create custom field data using scripting
- Plot distribution of field data
- Generate isosurfaces at specific field values
- Map field data onto isosurfaces to enhance understanding
- Visualize multiple slices of field data
- Orientation of the view along slice normals
- Partition fields into isolated segregates
- Analyze segregate size, radius and separation distributions

Scripting

- Environment for developing Perl scripts including syntax checking and debug tools
- New Perl script document with line numbering, bookmarks, and syntax coloring
- MaterialsScript API to control 3-D model documents:
 - Access to all properties on the Properties explorer
 - Manipulate geometry objects such as monitors, centroids etc.
 - Manipulate atoms and bonds
 - Calculate bonds, hydrogen bonds, and close contacts
 - Calculate conolly and solvent surfaces
 - Build polymers, crystals, surfaces, and layers
 - Use the symmetry tools such as SuperCell
 - Create and manipulate field data
- MaterialsScript API can be used to control the content of the study table
- Comprehensive on-line documentation of the API

Statistical Tools

- Univariate analysis gives mean, standard deviation, distribution data, etc.
- Data transformation tool
- Data standardization tool
- Generation of colored correlation matrices

Presentation

- Windows-standard page setup and output to printer
- Export of bitmap image creates high quality graphics for reports and presentations
- Export of trajectory files as video files in Microsoft .avi format