

# Materials Explorer™

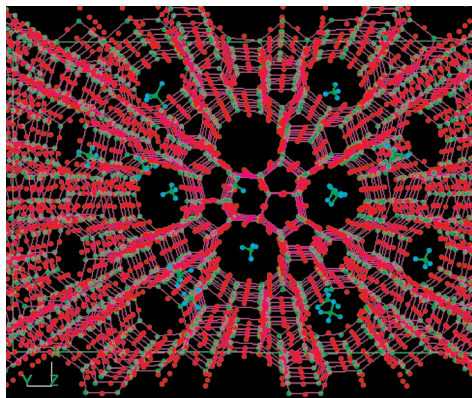
## Versatile Molecular Dynamics Package for Windows®

Materials Explorer is a computationally powerful molecular dynamics and Monte Carlo software package specifically designed to be an engineering tool to study materials with real-world applications.

### Features

#### Modeling capabilities

- ▶ *Crystal Builder* enables the study of inorganic solid state or molecular crystal systems.
- ▶ *Solution Modeler* makes the setup for randomized multi-component liquid or gas phase systems easy.
- ▶ *Layer Cell Modeler* for studying heterogeneous systems, (e.g. gas-solid interactions, organic bilayers, solid state grain boundaries, etc.)
- ▶ Structures built with **CAChe** or **WinMOPAC** molecular editors can be imported.
- ▶ Easy setup for molecular beam simulations to study crystal or epitaxial growth, surface adsorption, and surface destruction.
- ▶ Copy, cut and paste options makes it easy to model systems with defects or impurities.
- ▶ An optional client-server module is available for running high-performance calculations on vector or SMP UNIX servers.

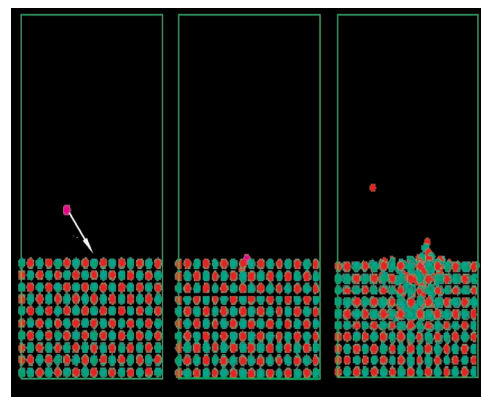


Adsorption of methane on zeolite

- ▶ *Potential Editor* manages the reading and editing of potential forms and parameters in the Potential Library.

- ▶ Time-dependent temperature and pressure control enables study of phase transitions and simulated annealing.

#### Scientific capabilities



MgO Substrate Sputtered by Ar Plasma

- ▶ Flexible simulation capabilities include
  - NEV, NTV, NPH and NTP using the Parrinello-Rahman-Nose methods.
  - SHAKE and MATRIX algorithm for bond constraints.
  - Periodic boundary conditions.
  - United atom model.
- ▶ Advanced algorithms for evaluation of interaction potentials dramatically improves computational efficiency.
- ▶ Application of external electric fields.
- ▶ Potential library comprised of numerous high-quality, published potentials, including two-body, three-body and embedded atom models.

#### Covering the Spectrum of Molecular Dynamics

- ▶ organics, polymers, biomolecules, metals, ceramics, semiconductors, etc.
- ▶ crystals, amorphous solids, liquids and gases (periodic boundaries)
- ▶ phase transitions, expansion, defects, compressibility, tensile strength, etc.

#### System Requirements

##### Operating System

Windows 98, Me, 2000 or XP

##### CPU

Pentium II or higher recommended

##### RAM

32MB or more recommended

##### Hard Disk

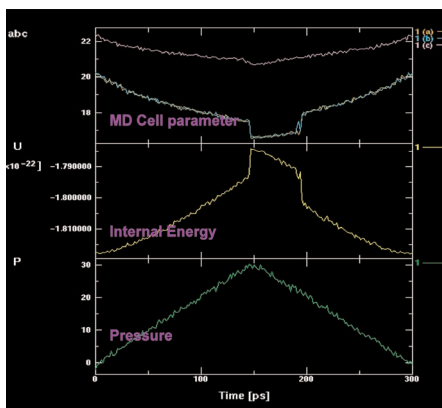
20MB for program plus 200MB or more recommended for data space

## Analysis capabilities

Materials Explorer can evaluate the following properties:

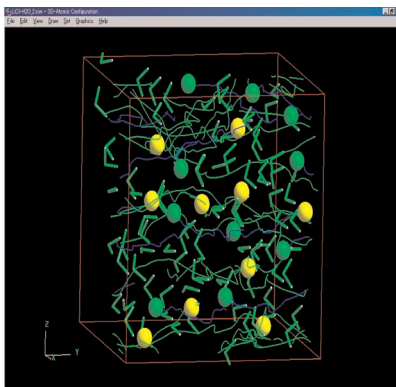
- Interference functions for X-ray and neutron diffraction.
- Pair-correlation and radial distribution functions.
- Mean square displacements and diffusion constants.
- Running integration number and Voronoi analysis for the characterization of amorphous solids.

Monitoring Module shows 2D graphs of temperature, pressure, internal energy and other properties monitored as a function of time.



Pressure-induced phase transition in AlPO4

Internal Coordinate Module allows user to view time-averaged value of selected internal coordinates.



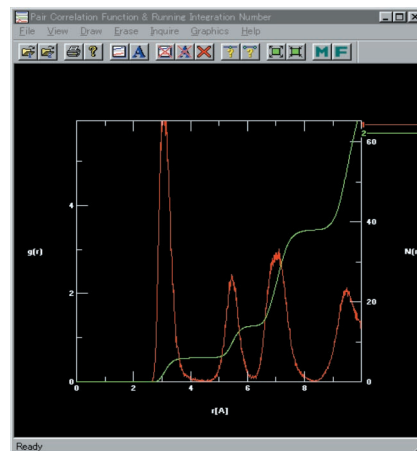
Aqueous LiBr subject to external electric field

3D Atomic Configuration Module displays snapshots, trajectories and animation of dynamical system.

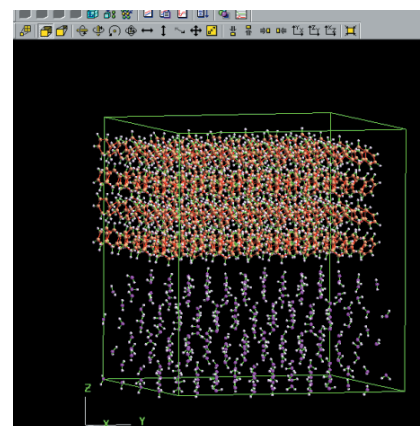
MSD Module calculates the Mean Square Displacement (MSD) from the output data. Afterwards, it displays a 2D graph of the MSD, the self-diffusion coefficient of each element, and the center of gravity of each molecule.

PCF Module calculates the Pair Correlation Function, Radial Distribution Function, and Running Integration Number, and displays the corresponding 2D graph.

Raw data involving all atom coordinates and velocities as a function of time can be saved in ASCII format for secondary analysis.



Pair-correlation function module



Layer-Cell Modeler easily creates simulation of water-benzene interface

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