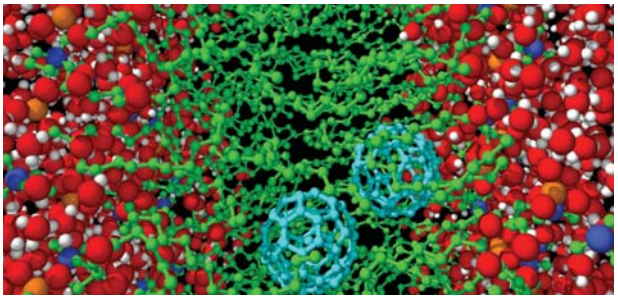
Wasatch Molecular INCORPORATED

WMI-MD Molecular Simulation Package

Molecular Dynamics Simulations Using WMI-MD™



WMI-MD is a molecular dynamics simulation package offered free by WMI that facilitates simulations and analysis of liquid, polymeric, crystalline and interfacial materials using the APPLE&P force field. Simple input/output file structure and the ability to modify and customize the code for a particular problem of interest make WMI-MD a very efficient, robust and attractive alternative to commercial packages.

WMI-MDs' capabilities include:

- simulations in NPT, NVT, NVE ensembles in cubic, orthorhombic, and fully flexible simulations cells;
- multiple time step and Langevin dynamics integrators;
- Ewald, particle mesh Ewald, and reaction field treatment of electrostatic interactions;
- ability to handle atomistic polarizable, non-polarizable and coarse-grained force fields expressed in analytical or numerical form.

Over the last decade WMI-MD has been extensively used in industry, national laboratories, and academia in the US and around the world to investigate a wide variety of materials and has resulted in more than 200 publications in peer reviewed scientific journals and several books.

Properties predicted using WMI-MD include:

STRUCTURAL & THERMODYNAMIC PROPERTIES

- equation of state
- free energy and enthalpy of solvation and vaporization
- crystal unit cell dimensions
- local and global molecular conformations

DYNAMIC AND TRANSPORT PROPERTIES

- rotational and translation diffusion
- ionic conductivity
- thermal conductivity
- viscosity
- coherent and incoherent dynamic structure factors
- NMR relaxation

MECHANICAL PROPERTIES

- mechanical and dielectric relaxation
- elastic constants
- bulk and shear modulus

WMI-MD is compatible with many commercial and published force fields including APPLE&P (see obverse).

Examples of materials investigated using WMI-MD + APPLE&P: ionic liquids; polymer melts, blends, and solutions; polymer and liquid electrolytes; nanocomposites; self-assembled nanostructures; surfaces and nanoparticles; biomolecules and biointerfaces; explosives and energetic materials.

For more information about WMI-MD, APPLE&P and other WMI products and services please contact us at info@wasatchmolecular.com or visit www.wasatchmolecular.com