

Atomistic Molecular Dynamics Simulations Using APPLE&P™



APPLE&P (ATOMISTIC POLARIZABLE POTENTIAL FOR LIQUIDS, ELECTROLYTES, & POLYMERS)

is an accurate and transferable many-body polarizable force field for classical molecular dynamics simulations of ionic liquids, liquid electrolytes, polymer electrolytes, and polymers. Building on 20 years of experience in developing force fields for atomistic simulations, APPLE&P is the newest generation, state-of-the-art force field that can be reliably applied and easily extended to a wide variety of complex materials.

Inclusion of many-body polarization effects allows APPLE&P to accurately capture electrostatic interactions in highly polar and polarizable environments, therefore allowing accurate prediction of a wide range of properties including:¹

STRUCTURAL & THERMODYNAMIC PROPERTIES

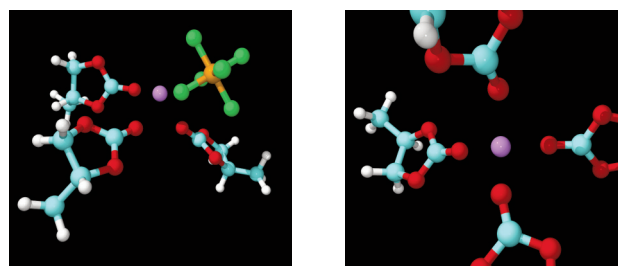
- equation of state
- free energy and enthalpy of solvation & vaporization
- crystal unit cell dimensions

DYNAMIC AND TRANSPORT PROPERTIES

- rotational and translation diffusion
- ionic conductivity
- thermal conductivity
- viscosity

MECHANICAL PROPERTIES

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



These material properties are relevant to a wide range of applications from lithium batteries, to separation membranes, to explosives and propellants. Recently, APPLE&P has demonstrated unprecedented accuracy for prediction of thermodynamic and transport properties of ionic liquids and liquid electrolytes. Great transferability of parameters makes APPLE&P easily extensible to a wide variety of different compounds without the need for expensive re-parameterization. APPLE&P is under continuous development and being extended to applications not listed above. Contact us today to discuss the latest developments and your needs at info@wasatchmolecular.com.

¹ The APPLE&P force field is distributed with the free open-source molecular simulation package, **LUCRETIVUS**. WMI offers technical support, consulting & training services, and custom modifications of this package to meet your needs.