materials design

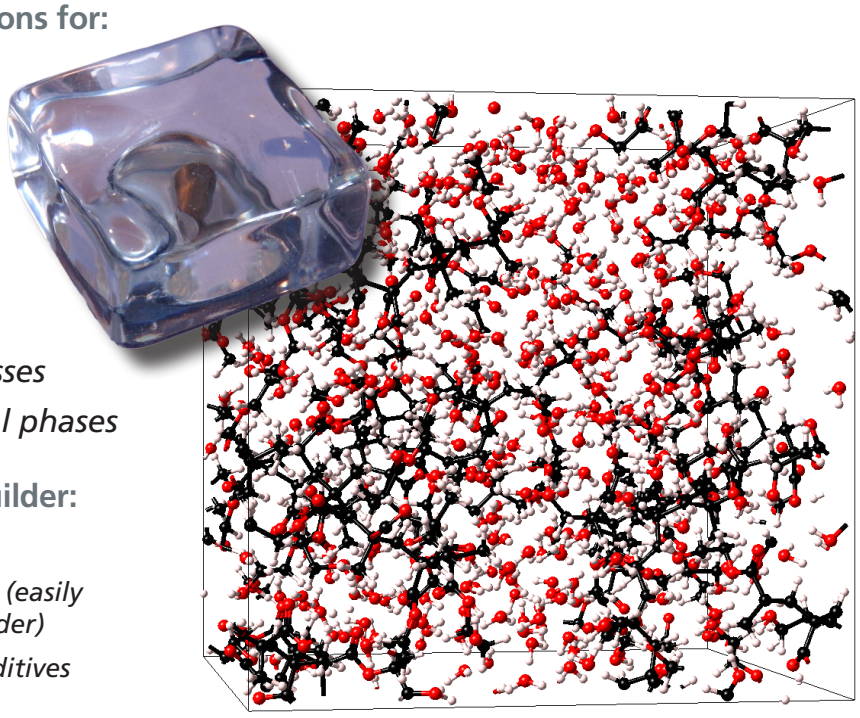
MedeA® Amorphous Materials Builder

The MedeA® Amorphous Builder lets you efficiently create condensed phase models based on system composition and target density.

In allowing you to focus on science, the MedeA® Amorphous Materials Builder eliminates the need for lengthy mixing and amorphization simulations, which for many polymeric and glassy systems can never sample all degrees of freedom due to the timescale of polymer backbone motion.

Create Statistically Realistic Configurations for:

- *Bulk polymers*
- *Polymer blends*
- *Polymer solutions*
- *Electrolyte systems*
- *Small molecule liquids*
- *Liquid mixtures*
- *Melts of mixed oxide inorganic glasses*
- *Coming Soon: Nematic liquid crystal phases*



Key Benefits of MedeA® Amorphous Builder:

- *Works well for:*
  - *Individual and multiple polymer chains (easily created with the MedeA® Polymer Builder)*
  - *Organic molecules such as solvents, additives and plasticizers*
  - *Inorganic material fragments*
- *Generate system configurations based on realistic sampling of the translational, rotational, and the conformational degrees of freedom of component species (subject to the constraint that the final model possesses complete translational periodic symmetry)*
- *Use output structures as the starting point for a range of condensed phase property evaluations for both polymer and small molecule organic systems*

Required MedeA® Modules

- *Core MedeA® Environment*
- *MedeA® Forcefield*
- *MedeA® JobServer and TaskServer*

Supported MedeA® Modules

- *MedeA® Polymer Builder*
- *MedeA® Mechanical Properties (MT)*
- *MedeA® LAMMPS-Thermal Conductivity*
- *MedeA® LAMMPS-Viscosity*
- *MedeA® LAMMPS-CED*

Visit our website www.materialsdesign.com or contact your local Materials Design office for further information.

Materials Design Inc., 343 West Manhattan Avenue, Santa Fe, NM 87501, USA
Telephone: +1 760 495-4924 • Fax: +1 760 897-2179 • E-mail: info@materialsdesign.com • www.materialsdesign.com