MedeA Amorphous Materials Builder

A Versatile Non-crystalline Model Building Tool

At-a-Glance

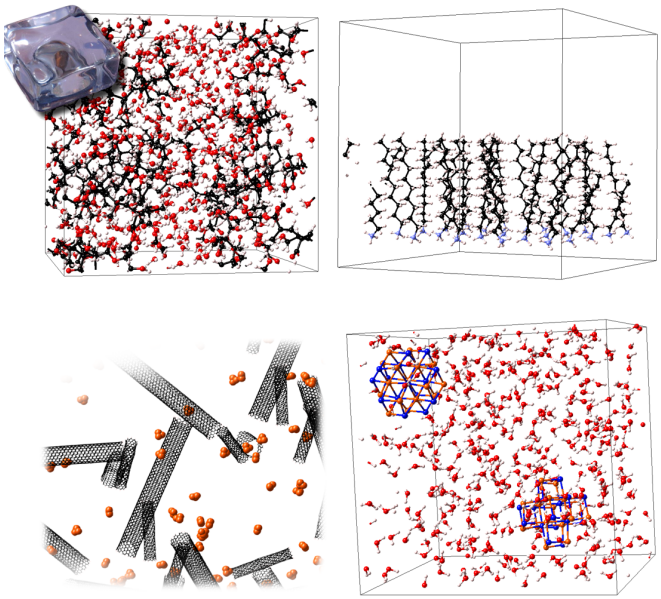
The *MedeA* ®[1] *Amorphous Materials Builder* enables the efficient creation of disordered condensed phase models based on system chemical composition and target density. The Builder eliminates the need for lengthy mixing and amorphization simulations, and allows you to focus on the science.

Glassy materials in general, like all polymeric systems in *any* physical state, are unable to sample all degrees of freedom using molecular dynamics simulation alone, due to the timescale of diffusive and/or polymer backbone motions. Accordingly, the Amorphous Materials Builder employs a Monte Carlo approach (based on realistic sampling of the translational, rotational, and conformational degrees of freedom of component species) to generate configurations typical of those found in real amorphous materials at or close to equilibrium.

Key Benefits

- Creates Realistic Configurations for:
  - Bulk polymers
  - Polymer blends and solutions
  - Uncured thermosets
  - Molecular fluids
  - Multicomponent liquid mixtures
  - Electrolyte systems
  - Nanoparticle-fluid or nanoparticle-polymer mixtures
  - Melts of mixed oxide glasses
  - Surfactant/Lipid monolayers and bilayers
  - Nematic liquid crystal phases
  - Layered interfacial systems

- Provides output structures directly suitable for use as the starting point for a range of condensed phase property evaluations for small molecule organic, polymeric, and amorphous inorganic systems, using the LAMMPS, GIBBS or VASP engines.



'The range of model types that the Amorphous Materials Builder can create is impressive. This makes it an ideal builder for use in any materials modeling group working on projects involving polymers, fluids, mixtures and interfacial systems, which sometimes contain multiple components including organic material, ionic species and inorganic solids all within the same system.'

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

Key Features

- Seamlessly use with other *MedeA* builders, such as the Molecular, Mesoscale and Polymer Builders, and Stacked Layer ('multilayer') Builder
- Supports insertion of molecules as rigid or flexible species, allowing exploration of restricted or all degrees of freedom within individual component molecules
- Optionally use the builder 'sequentially' to insert molecules into either amorphous or crystalline models (e.g. glassy and rubbery polymer, or zeolites), as required when studying behavior of small penetrant molecules
- Incorporates additional capabilities for controlling the placement of specified atoms and biasing orientation of sections of molecules, thereby facilitating generation of models of partially-ordered materials such as surfactant monolayers
- Designed to be used both interactively and in *MedeA-HT* flowcharts for use where many configurations must be sampled to obtain meaningful averages over a statistical ensemble

Required Modules

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

Related Modules

- *MedeA Polymer Builder*
- *MedeA Mesoscale Builder*
- *MedeA HT-Launchpad*
- *MedeA HT-Descriptor*
- *MedeA CED*
- *MedeA Thermal Conductivity*
- *MedeA Viscosity*
- *MedeA Mechanical Properties (MT)*

Find Out More

Learn more about how *MedeA Amorphous Materials Builder* has been used in a wide variety of materials research projects by viewing the following webinars:

- Computational Polymer Science: Atomistic Modeling Tools and Materials Applications
- Predicting Elastic Properties Using Ab Initio and Forcefield Based Simulations
- Explore the MedeA 2.22 atomistic simulation environment
- High Value from High Throughput in the MedeA Environment

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