

# MedeA Polymer Builder

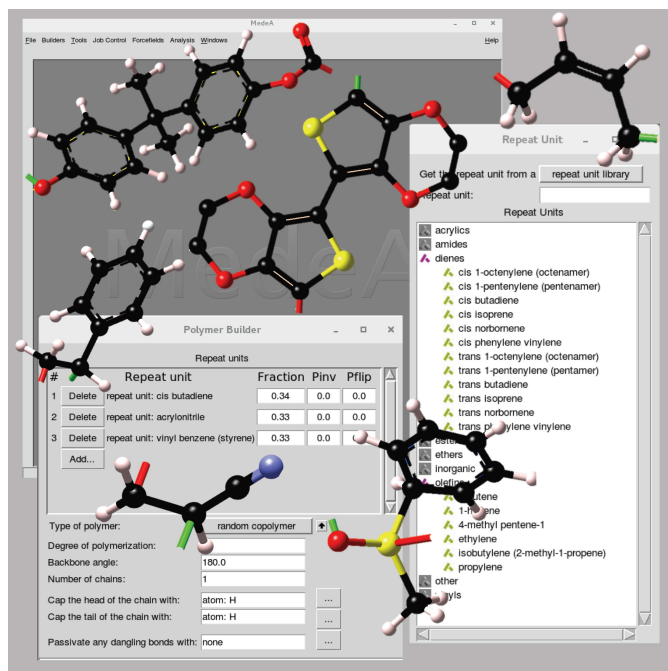
A Foundation Tool for Atomistic Model Building

## At-a-Glance

The MedeA<sup>®</sup><sup>1</sup> Polymer Builder creates models of isolated polymer chains, providing a foundation for building more complex models. Examples include bulk polymers, blends, solutions, or multiphase systems incorporating one or more interfacial regions. An extensive library of polymer repeat units is provided, enabling most common polymer structures to be created with minimal user input. Whenever custom repeat units are required, these may be sketched and defined with just a few mouse clicks.

## Key Benefits

- Quickly builds models of individual homopolymer and copolymer chains
- Works with an extensive built-in repeat unit (RU) library, or with any custom-built unit
- Uses RUs as input to the rapid polymer property prediction tool MedeA P3C
- Provides input for building more complex polymer systems, such as bulk polymers, thin films, crosslinked models, solutions, and blends



*‘Since so many products and devices essential to modern lifestyles contain polymers in one form or another, it is often necessary to be able to incorporate these materials into our modeling projects. Using the \*MedeA Polymer Builder\* has transformed this once tedious model building activity into a routine exercise requiring minimal effort, enabling us to concentrate on the fundamental scientific aspects of materials exploration work.’*

## Key Features

- Extensible library with over 120 common repeat units
  - Acrylics
  - Amides
  - Carbohydrates and Saccharides
  - Dienes
  - Esters

The MedeA Polymer Builder creates polymer models from specified repeat units and polymerization information. Create homopolymers with two clicks from a library of more than 120 repeat units, and generate complex copolymers with additional rules and appropriate sequence definitions. If you need to define terminations or the backbone angle, you have the freedom to tune the standard defaults.

The MedeA Polymer Builder is simple for basic construction, yet sophisticated for even the most demanding builds. The results consist of quality polymer models based on more than 25 years of experience in computational polymer science.

<sup>1</sup> MedeA and Materials Design are registered trademarks of Materials Design, Inc.

- Siloxanes
  - Olefins
  - Vinyls
- Flexible repeat unit definition for any monomer
- Use for creating both fully atomistic and coarse-grained mesoscale models
- Handling of any required tacticity
  - Isotactic
  - Syndiotactic
  - Atactic
- Full control of polymer repeat unit orientation - head-to-head, head-to-tail, or random
- Alternating, block, and random copolymer capabilities employing user defined probabilities
- Generation of an arbitrary number of chains
- Define chain lengths, tacticity, torsion angles, and handling of terminal groups

## Characteristics & Uses

- Create any desired repeat unit with the *MedeA Molecular Builder*
- Use the models that *MedeA Polymer Builder* creates to prepare bulk models for atomistic simulations of physical properties including:
  - Density and PVT Properties
  - Cohesive Energy Density (CED)
  - Adhesion
  - Surface and Interfacial tension
  - Thermal Conductivity
  - Diffusivity
  - Gas and Moisture Sorption

## Required Modules

- *MedeA Environment*

## Related Modules

- *MedeA Amorphous Materials Builder*
- *MedeA Mesoscale Builder*
- *MedeA HT-Launchpad*
- *MedeA HT-Descriptor*
- *MedeA Diffusion*
- *MedeA Surface Tension*
- *MedeA Thermal Conductivity*
- *MedeA Mechanical Properties (MT)*
- *MedeA P3C*
- *MedeA Thermoset Builder*

## Find Out More

Learn more about building polymer chains and creating custom repeat units by viewing the following online tutorials:

- [Building polymers : How to Build a Polymer](#)
- [Creating custom repeat units: How to Build a Polymer with Customized Repeat Unit](#)