



materials design®

# MedeA® Thermoset Builder

Densely crosslinked thermosetting polymers are essential components of a wide variety of modern materials systems with applications ranging from advanced aerospace and automotive composites, electronic and optical device fabrication, dental restoration and commodity construction and architectural design materials. The MedeA® Thermoset Builder combines methods developed in the 1980's and early 1990's for predicting network polymer topologies<sup>[1-3]</sup> with proven strategies for preparing well-equilibrated, atomistic-level structures of densely packed amorphous polymers in order to create strain-free molecular models with experimentally observed crosslink densities.

## Key Benefits of MedeA® Thermoset Builder: Create Realistic Models of:

■ **Full integration into MedeA® Flowcharts, for batch processing, property averaging and straightforward combination with:**

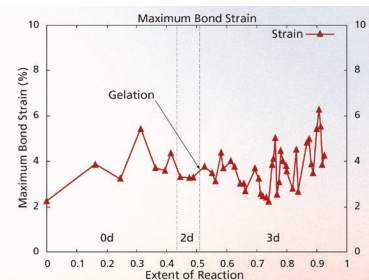
- ▶ MedeA® Amorphous Builder to create uncured starting materials
- ▶ MedeA® LAMMPS for generation of dynamics trajectories
- ▶ Property calculation modules for prediction of density (shrinkage), mechanical properties and thermal conductivity using accurate forcefields

■ **Rigorous monitoring of material characteristics during crosslinking**

- ▶ Evolution of network structure and gel point
- ▶ Bond strain
- ▶ Automatic defect detection (for avoidance of unphysical ring catenations)

■ **Ability to study a wide variety of combinations of resins and curing agents, with or without the presence of added solvent**

- Epoxies
- Bismaleimides (BMI, polyimides)
- Polyurethanes
- Thermosetting acrylics
- Polyesters (alkyds)
- Urea / Phenol / Melamine-Formaldehyde plastics



DDCyM

**DDS**

DETDA

IPD

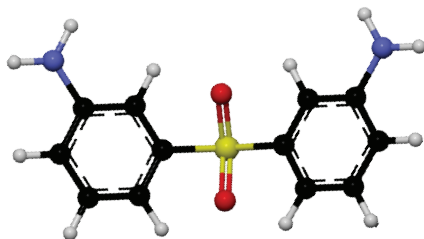
J-EDR148

J-T408

MPD

MXD

TEPA



## Required MedeA® Modules

- MedeA® JobServer and TaskServer
- MedeA® Amorphous Materials Builder
- MedeA® Forcefield

## Recommended MedeA® Modules

- MedeA® Mechanical Properties (MT)
- MedeA® LAMMPS Thermal Conductivity

### References:

- [1] L.Y. Shi, Y.K. Leung and B.E. Eichinger, *Macromolecules* 18, 983 (1985).
- [2] V. Galiatsatos and B.E. Eichinger, *J. Polym. Sci. Polym. Phys. Ed.* 26, 595 (1988).
- [3] O. Akgiray, *Makromol. Chem. Makromol. Symp.* 76, 211 (1993).

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