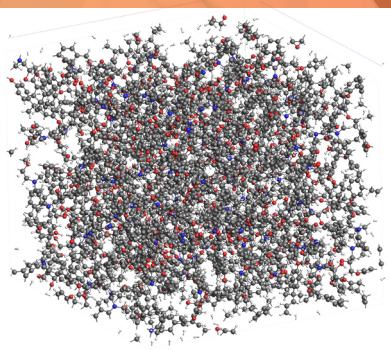
Polymers
with the Amsterdam Modeling Suite

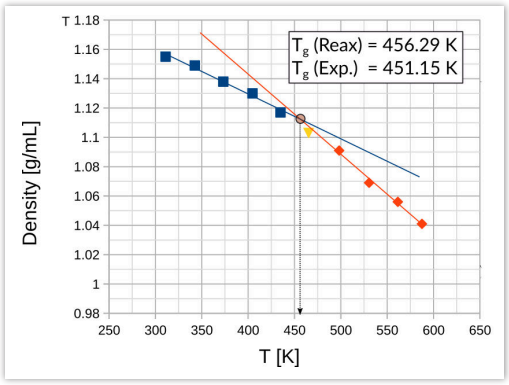


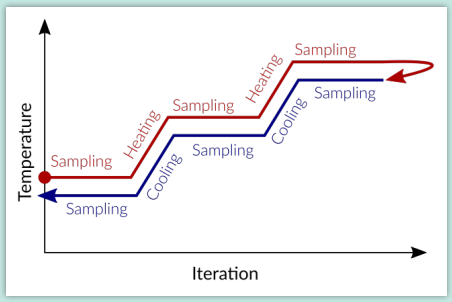
Understand mechanisms and processes, at the atomic scale

Molecular modeling and simulations play a crucial role in the field of polymer science and engineering. These simulation methods are essential for predicting and explaining various aspects of structures, dynamics, thermodynamics, and material properties at both microscopic and macroscopic levels.

What can you compute with AMS?

- Mechanical properties (stress tensors, stress-strain curves, coefficient of thermal expansion, glass transition temperature)
- Degradation and healing pathways
- Redox potentials, charge mobility
- Thermodynamic properties of mixtures (activity, vapor pressures, solubilities, partition coefficients, Flory-Huggins parameters)
- Optical properties



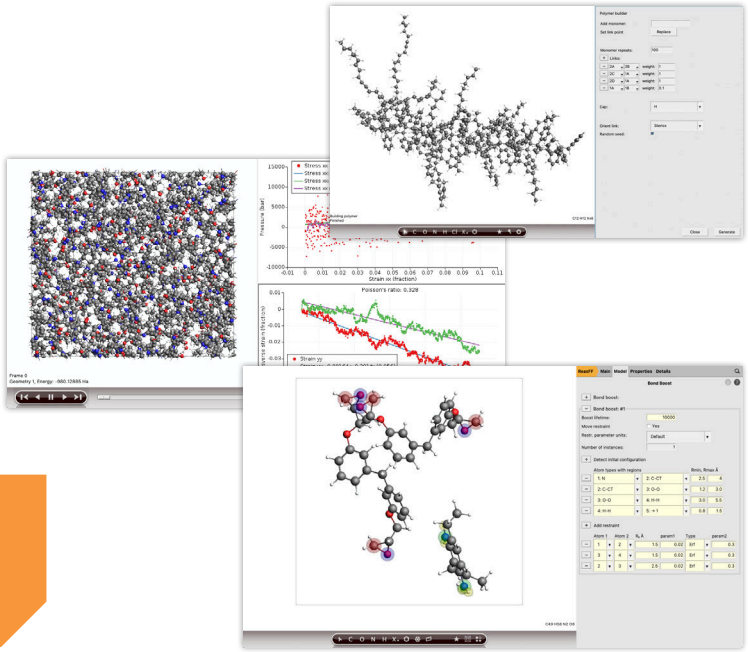


Key methods for polymer modeling

- √ ReaxFF, Machine Learning Potentials, UFF
- √ COSMO-RS for thermodynamic properties (solvents and mixtures)
- √ ADF, BAND and DFTB

Tools and analysis for polymer modeling

- Polymer builder, and polymer database
- Bond boost to accelerate reactive polymerization, cross-linking
- Automatic mechanical properties extractor (Young's modulus, Poisson's ratio)
- Versatile MD deformation tool
- Simulated annealing to generate amorphous structures



SCM
Software for Chemistry & Materials

Explore polymers with AMS

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SCM
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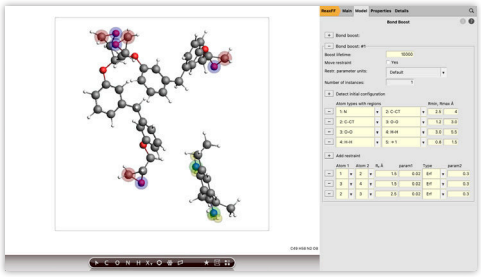
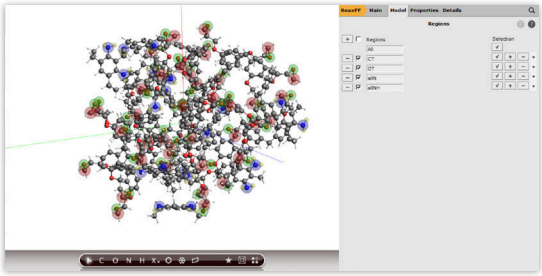
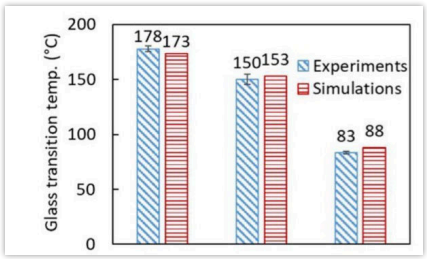
Understand and predict polymer cross-linking

Because simulating reactions on realistic time scales is computationally expensive, an accelerated simulation method was developed, which is particularly suitable for reactive molecular dynamics simulations. With this bond boost, you can generate realistic atomistic models of epoxy polymers for which the mechanical properties can then be simulated.







Methods and results

Generating realistic crosslinking polymers with the Amsterdam Modeling Suite is intuitive with the graphical user interface. Just define the reactive atoms and set up the parameters for the bond boost. Scale-up the process to hundreds of moieties and obtain realistic bulk structures of cross-linked polymers for different combinations. From there, you can anneal the system to extract the glass transition temperature and coefficients of thermal expansion, or you can deform it to compute its mechanical properties.

"What I really like about the Amsterdam Modeling Suite is that the programs were clearly written by chemists for dealing with real chemical problems. A great suite of programs!"

– Roald Hoffmann, Nobel Laureate

About SCM

Scientists at SCM are passionate about making computational chemistry work for you. Our mission is to develop powerful, easy-to-use software for your research and development needs. We love to discuss your research and learn how we can serve you better in the future.

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