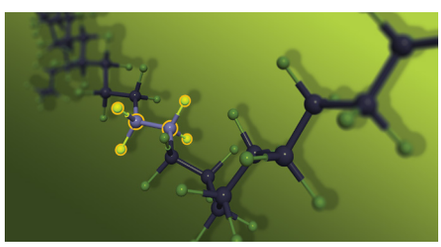
SYNOPSYS®

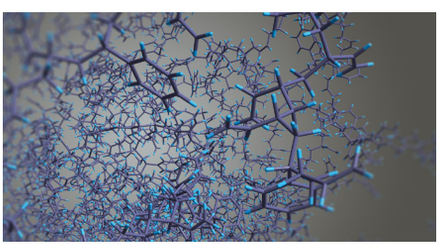
Polymer Simulations with QuantumATK

QuantumATK atomic-scale modeling software is used to design polymers with improved thermo-mechanical, thermal conductivity and optical properties within R&D of areas such as photoresist, transparent polymers, rubber-like polymers for tire industry and thermoset polymers for insulation industry. Polymer building and equilibration tools in QuantumATK provide reliable polymer models, which can then be simulated using fully automated workflows, powered by a highly scalable MPI parallelized molecular dynamics (MD) engine.

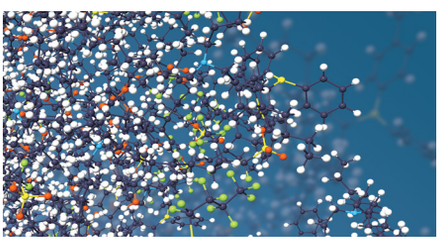
Supported Polymer Systems



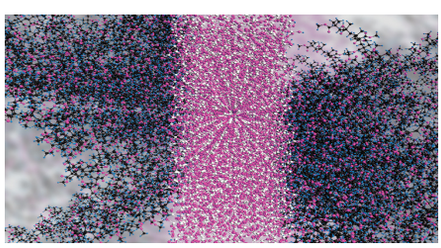
Linear homo-polymers, co-polymers and polymer blends. Polymers with specific chemical composition.



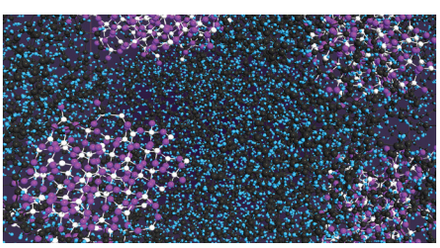
Polymer/Polymer blends. Example: Poly(butadiene-co-styrene) melt.



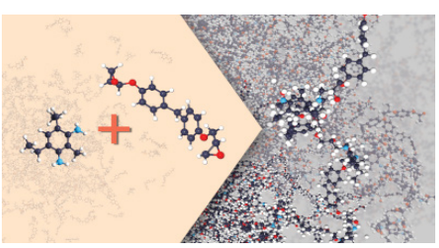
Polymer/Molecule blends. Example: Photo acid generator (PAG) molecules in PMMA matrix.



Polymer/Polymer and Polymer/Inorganic interfaces. Example: Polymer/SiO_2 interface.

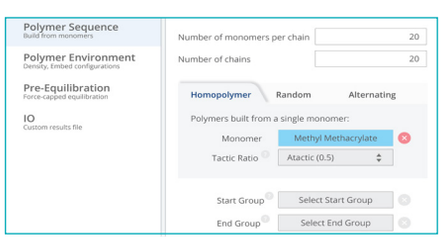


Polymer/Nanoparticle composites. Example: Polymer melts with SiO_2 nanoparticles.

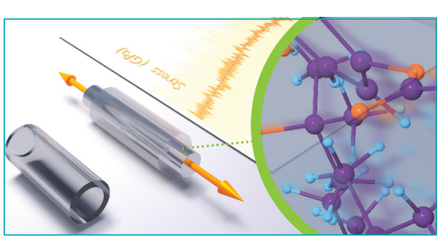


Polymers with cross-linked or 3D network structures. Example: Amine-epoxy cross-linking reaction.

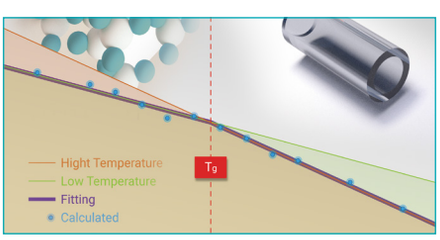
Key Benefits of QuantumATK



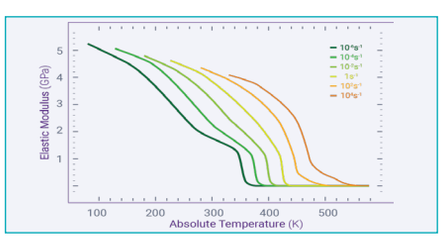
Advanced GUI polymer builder



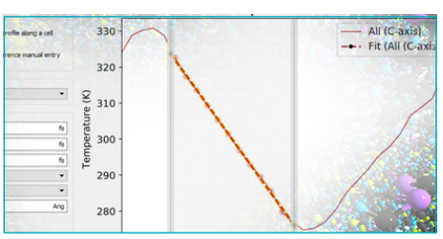
Stress-strain simulations (Young's modulus)



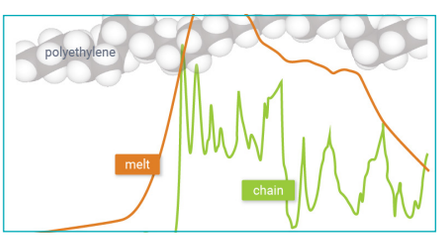
Glass transition temperature studies



Elastic modulus at different strain rates



Thermal conductivity studies



Optical properties

www.synopsys.com/silicon/quantumatk.html

Polymer Simulation Workflows in QuantumATK

Builder

- Extremely flexible and user friendly
- Full control of tacticity (iso-, syndio-tactic & atactic), monomer composition & end groups
- Large ready-to-use monomer and end-group database, add custom monomers
- Interface to embed single molecules, nanoparticles, surfaces
- Automatic assignment of monomer tags to define monomer linking reactions
- Monte Carlo builder for polymer melts. GUI and Python support for automation
- Tools for building polymers with cross-linked or 3D network structures

Parameter Setup

- More than 300 pre-defined parameters sets (including Tersoff, (M)EAM, ReaxFF, ionic, and bonded force fields, etc.)
- Automatic potential generation for DREIDING, UFF and OPLS-AA
- Charge equilibration using QEq and ReaxFF methods

Polymer Equilibration Methods

- Force-capped equilibration tools for initial equilibration
- Single-Chain Mean-Field (SCMF) equilibration
- Energy minimization for relaxing the polymer system
- 21 step polymer equilibration protocol (alternating NVT and NPT)
- Save and share customized protocols

Simulation Methods

- Molecular Dynamics (MD) in the NVE, NVT, and NPT ensembles
- Time-stamped Force-bias Monte Carlo (TFMC) simulation for enhanced equilibration and simulating events over longer timescales
- Non-equilibrium momentum exchange for modelling heat transfer in polymers

Advanced Techniques

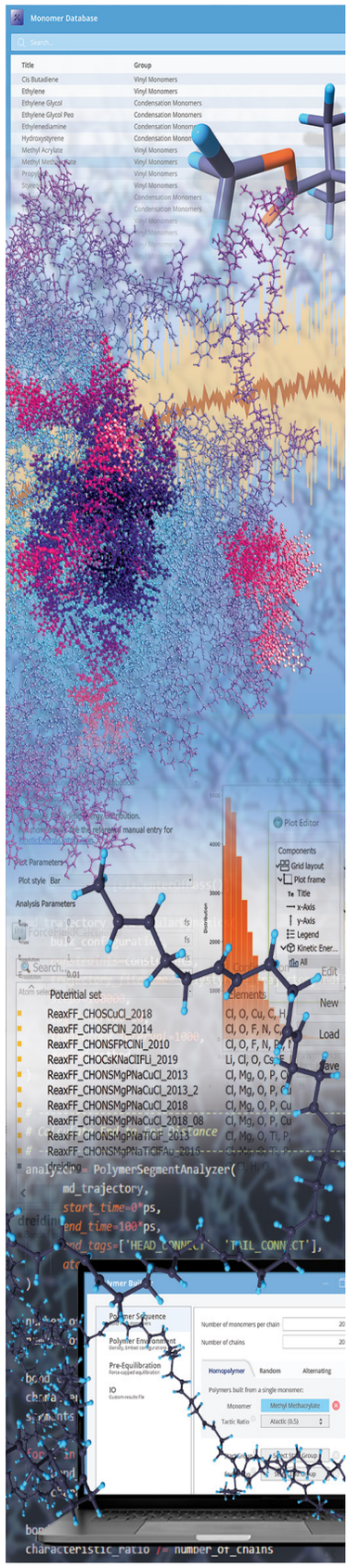
- United atoms and coarse-grained polymers to speed up simulations
- Hook functions to implement customized simulation techniques and measurements in molecular dynamics
- Metadynamics simulations via interface to the PLUMED package

Analysis Tools

- Advanced analysis tools in the GUI: glass transition temperature analyzer, temperature profile for heat transport, end-to-end distances, free-volume, etc.
- Interactive MD trajectory analysis and movie generation

High Performance

- Highly scalable MPI parallelized molecular dynamics engine



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