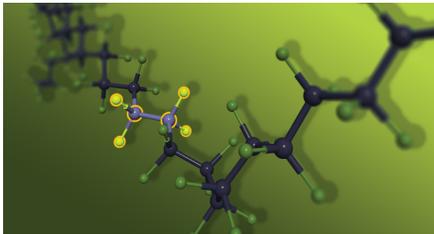


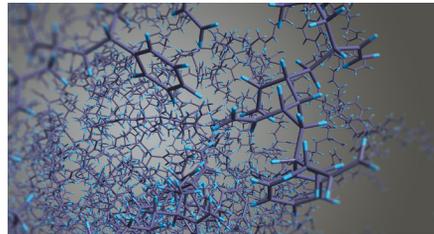
Polymer Simulations with QuantumATK

QuantumATK is a complete and fully integrated software suite for atomic-scale modeling of polymers, professionally engineered using state-of-the-art scientific and software-engineering methods. It combines the power of a Python scripting engine with the ease-of-use provided by an intuitive graphical user interface (GUI).

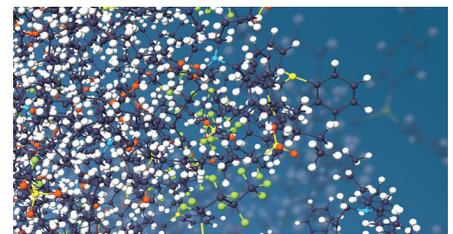
Supported Polymer Systems



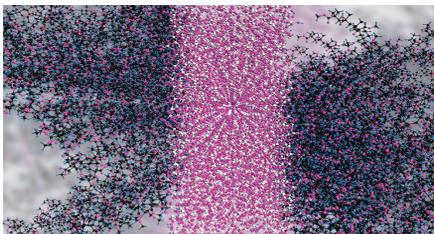
Linear homo-polymers, co-polymers and polymer blends.



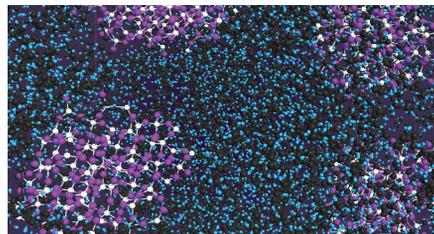
Polymer/Polymer blends. Example: Poly(butadiene-co-styrene) melt.



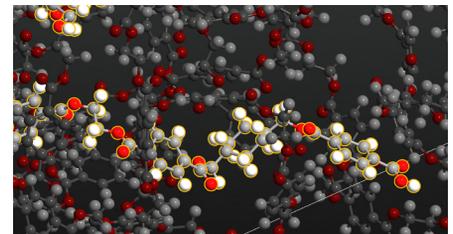
Polymer/Molecule blends. Example: Photo acid generator (PAG) molecules in PMMA matrix.



Polymer/Polymer and Polymer/Inorganic interfaces. Example: Polymer/SiO₂ interface.

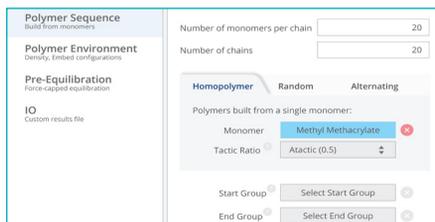


Polymer/Nanoparticle composites. Example: Polymer melts with SiO₂ nanoparticles.

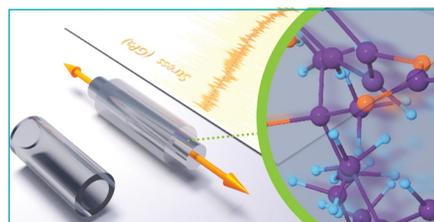


Polymers with specific chemical composition. Example: Poly(ethylene terephthalate) glycol-modified with cyclohexane dimethanol.

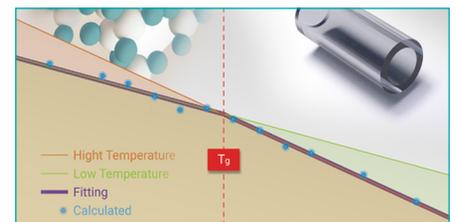
Key Benefits of QuantumATK



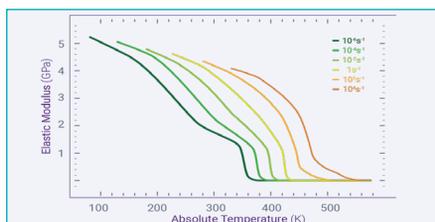
Advanced GUI polymer builder



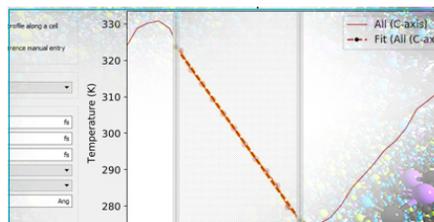
Stress-strain simulations (Young's modulus)



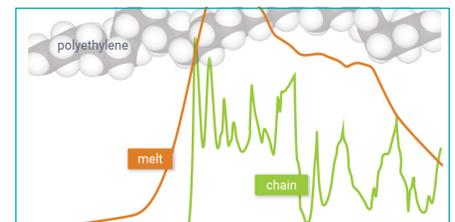
Glass transition temperature studies



Elastic modulus at different strain rates



Thermal conductivity studies



Optical properties

Polymer Simulation Workflows in QuantumATK

Builder

- ▶ Extremely flexible and user friendly
- ▶ Full control of tacticity (iso-, syndio-tactic and atactic), monomer composition, and end groups
- ▶ Large ready-to-use monomer and end-group database
- ▶ Possibility to add custom monomers
- ▶ Interface to embed single molecules, nanoparticles, surfaces
- ▶ Monte Carlo builder for polymer melts. GUI and Python support for automation

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 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

- ▶ 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, such as glass transition temperature analyzer, temperature profile for heat transport
- ▶ Interactive MD trajectory analysis and movie generation

High Performance

- ▶ Highly scalable MPI parallelized molecular dynamics engine

The image displays a vertical stack of screenshots from the QuantumATK software interface. At the top, the 'Monomer Database' window is visible, featuring a search bar and a table with columns for 'Title' and 'Group'. Below this is a 3D ball-and-stick model of a polymer chain. The middle section shows a 'Plot Editor' window with a histogram and various plot settings. At the bottom, the 'Polymer Builder' window is shown, containing fields for 'Polymer Sequence', 'Pre-Equilibration', and 'Homopolymer' options, along with a 'Tactic Ratio' dropdown menu.



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