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

www.synopsys.com/silicon/quantumatk.html
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