SYNOPSYS®

Simulations of Polymers Using QuantumATK

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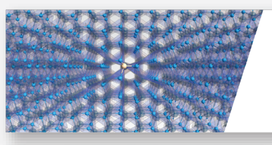
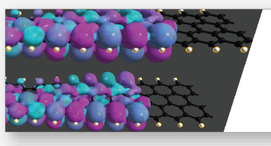
QuantumATK Platform[1,2]

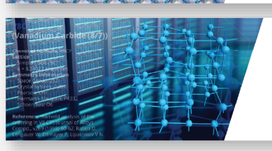
- NanoLab GUI:



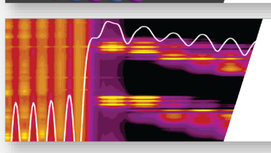
Atomic 3D Builder
Set Up Structures and Devices



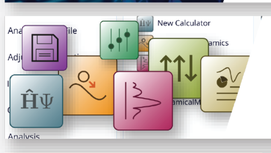
View Results
Visualize 2D and 3D Data



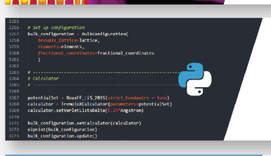
Databases
Import Ready-to-Use Structures



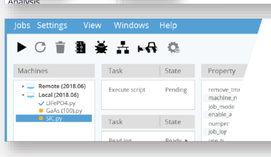
Advanced Analysis
Use Flexible Tools for Complex Studies



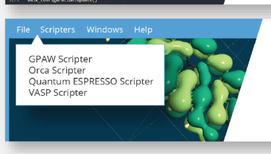
Set Up Calculations
Prepare Input Files with Script Generator



Python Scripts
Write Your Own Custom Scripts



Job Manager
Execute and Manage Local & Remote Jobs



NanoLab Links
Link to External Simulation Engines

- Simulation Engines:

DFT-LCAO → 10^3 - 10^4 atoms

DFT-PlaneWave → 10^2 - 10^3 atoms

Semi-Empirical → 10^5 atoms

ForceField → 10^5 - 10^7 atoms

NEGF, SGF device and surfaces

Polymer Builder

Builders
- Monte Carlo builder for polymer melts

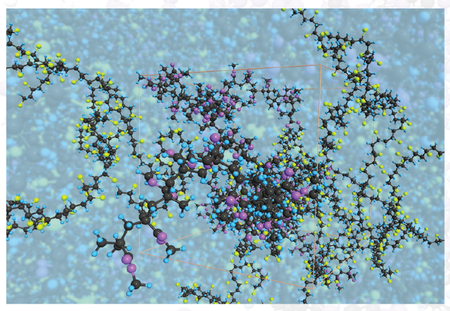
Equilibration
- Force-capped equilibration tools for initial equilibration
- Single-Chain Mean Field (SCMF) equilibration
- Energy minimization for relaxing thepolymer system

Simulation Methods
- Molecular Dynamics (MD) in the NVE, NVT, NPT ensembles
- Time-Stamped Force-Bias Monte Carlo (TFMC) for enhanced equilibration and simulating events over longer timescales
- Non-equilibrium momentum exchange for modelling heat tranfer in polymer systems

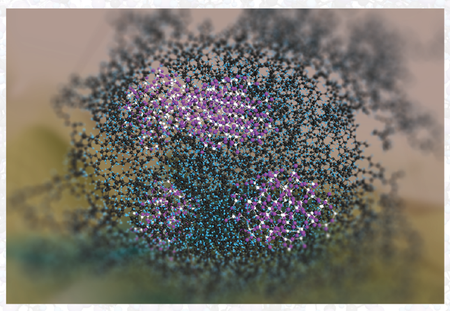
Advanced Techniques
- Hook functions to implement customized simulations and measurements in MD
- Metadynamic simulations through an interface to the Plumed package

Polymer Builder GUI
- Linear homo-, co-polymers, and polymer blends
- Control tacticity, end groups etc.
- Embed: Small molecules, nano-particles, surfaces
- Ready-to-use monomer and end-group database

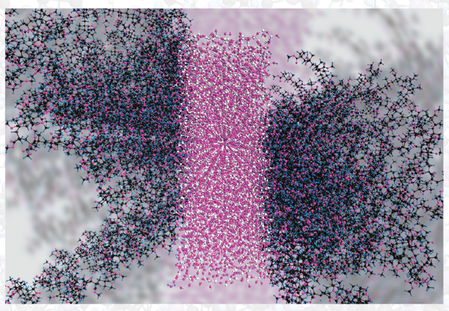
Application Examples

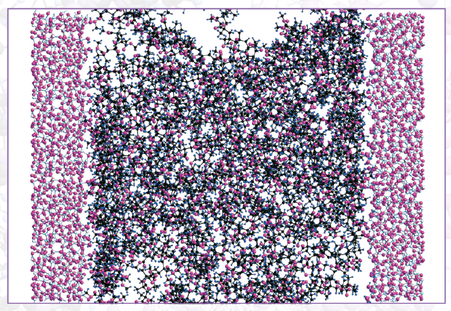


PVC/PMMA blend: Solubility, Flory-Huggins coefficients.



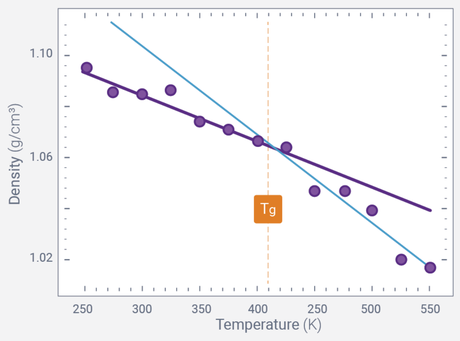
SiO_2 nano-particles in poly-butadiene matrix.





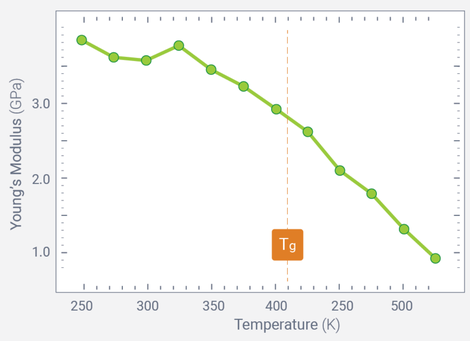
Realistic interface model: am-SiO_2 surface, OH-terminated / PMMA: (DREIDING / QEq charges). Strain applied along surface normal, interface system starts failing in the polymer layer (not at the interface).

Glass Transition

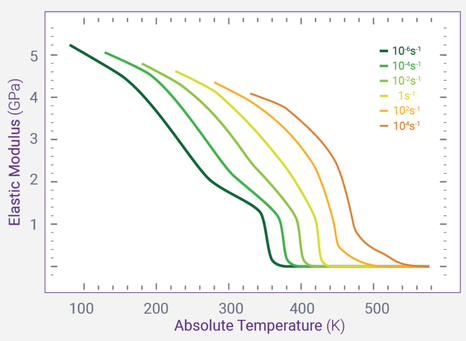


Glass transition close to Experiment: 410K (380K).

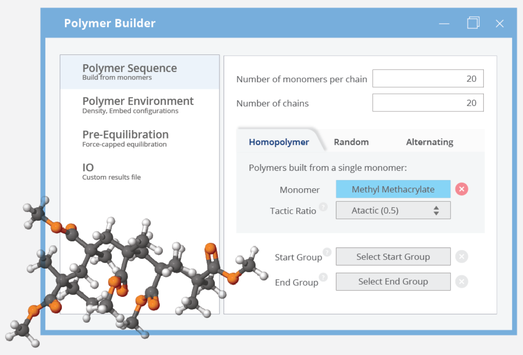
Young's Modulus: PMMA Melt (OPLS-aa)



Temperature-dependent Young's modulus. Simulated strain-rate: 0.1/ns.



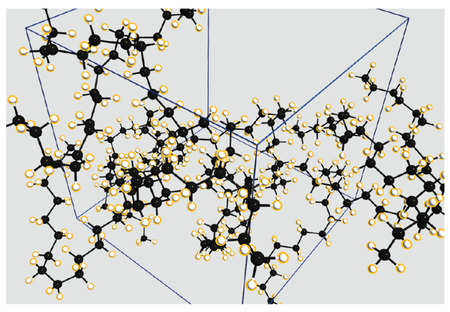
Model prediction at different strain rates, based on experimental results[3].

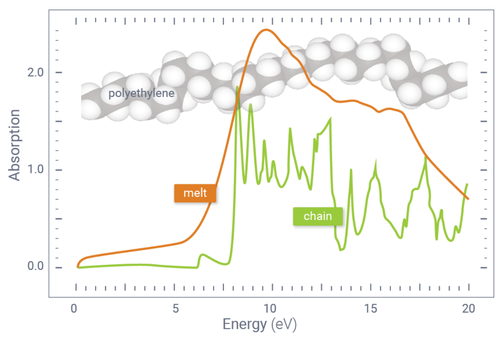


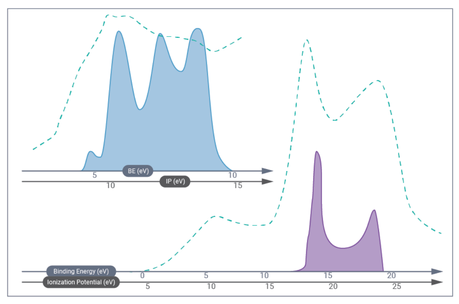
Poly(Methyl MethAcrylate) (PMMA)

Optical Properties of Polymers

Combine FF and ab-initio







Comparison of experimental spectrum with theoretical DOS

- Create small polymer melts using polymer builder and FF-equilibration.
- Take representative configuration and calculate electronic structure with ab-initio.
- Optical Spectrum based on Hückel-model and Kubo-Greenwood susceptibility.
- Agreement with experiment much better than for single straight chain model[4].

References

[1] QuantumATK, version P-2019.03, Synopsys QuantumATK (synopsys.com/silicon/quantumatk.html).
[2] QuantumATK: An integrated platform of electronic and atomic-scale modelling tools, Søren Smidstrup *et al.*, J. Phys.: Condens. Matter (2019).
[3] A.D. Mulliken, M.C. Boyce / Int. J. Solids and Structures 43 (2006) 1331–1356
[4] J. Delhalle et al. J. Chem. Phys. 60 (1974) 595