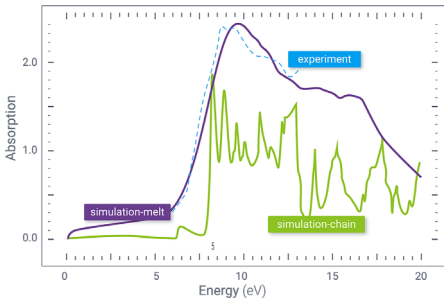
SYNOPSYS®

Optical Properties Simulations with QuantumATK

QuantumATK is a complete and fully integrated software suite for atomic-scale modeling of emerging bulk, 2D materials, and nanostructures. QuantumATK enables simulation and advanced analysis of a large range of optical and electro-optical parameters through fully automated workflows in NanoLab GUI.

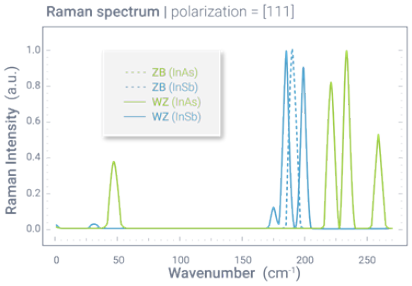
Key Benefits of QuantumATK



Material Properties

- Refractive indices, extinction coefficients, reflectivity, susceptibility, optical conductivity
- Optical spectrum including interband and intraband contributions

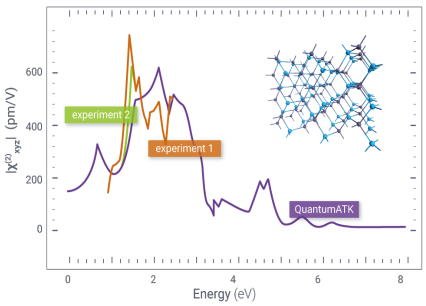
Example: Optical spectrum for polyethylene polymer melt structure vs. traditional chain of monomers.



Spectroscopy

- Raman spectrum:
  - Polarization dependent for one or multiple angles between incoming and scattered light
  - Polarization averaged spectrum
- Infrared spectrum

Example: Raman spectra for zinc-blende (ZB) and wurtzite (WZ) phases of InAs and InSb.



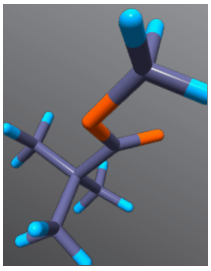
Nonlinear Optics

- Second harmonic generation (SHG) susceptibility
- Electro-optical tensor

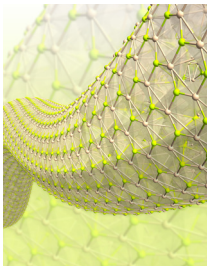
Example: SHG susceptibility for GaAs

Types of Systems

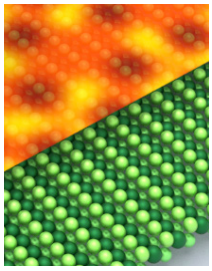
molecules



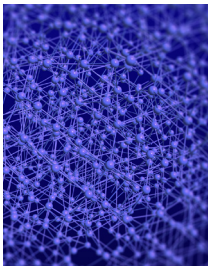
nanostructures



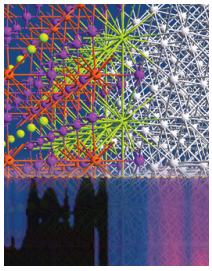
2D



bulk



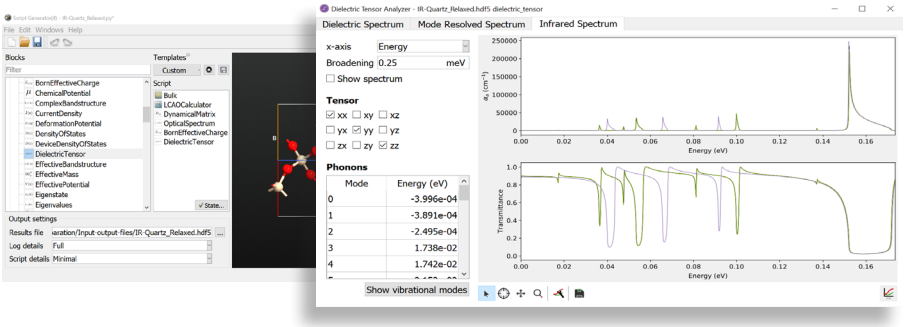
interfaces



poly(crystalline), amorphous, alloys

Key Advantages

- Large range of optical and electro-optical parameters
- Fully automated workflows in NanoLab GUI to reduce the chance of errors and TAT
- Advanced features for polar materials (ionic contribution, temperature dependence through electron-phonon coupling)



www.synopsys.com/silicon/quantumatk.html

Workflow for Efficient and Accurate Simulation of Optical Properties

3D Builder

- Build molecules, crystals, nanostructures, etc. using advanced selection and move tools
- Use 1st party plugins for setting up interfaces, grain boundaries, nanowires, nanoparticles, polycrystals, alloys, amorphous structures, cleave surfaces
- Import ready-to-use structures from the internal NanoLab database and online databases such as Crystallography Online Database and Materials Project or create your own databases

Simulation Set Up

- Use NanoLab GUI scipter to set up calculator settings and workflows for calculating optical properties, save them as templates
- Edit input files (python scripts) using the NanoLab editor

Structural Optimization & Vibrations

- Choose between Quasi-Newton LBFGS and FIRE methods for geometry and unit cell optimization (forces and stress)
- Compute phonon vibration modes using an automated DynamicalMatrix workflow
- Choose between DFT-LCAO and Force Field calculators

Optical Properties Simulations

- Choose between DFT-LCAO (all optical properties) and DFT-PlaneWave calculators (optical spectrum and SHG susceptibility)
- Employ a method for obtaining accurate bandgaps: (DFT+1/2 or HSE Hybrid)
- Calculation of susceptibility derivatives, Born effective charges and required optical properties are automatically included in a workflow where needed
- Use advanced features for polar materials (ionic contribution, temperature dependence through electron-phonon coupling)

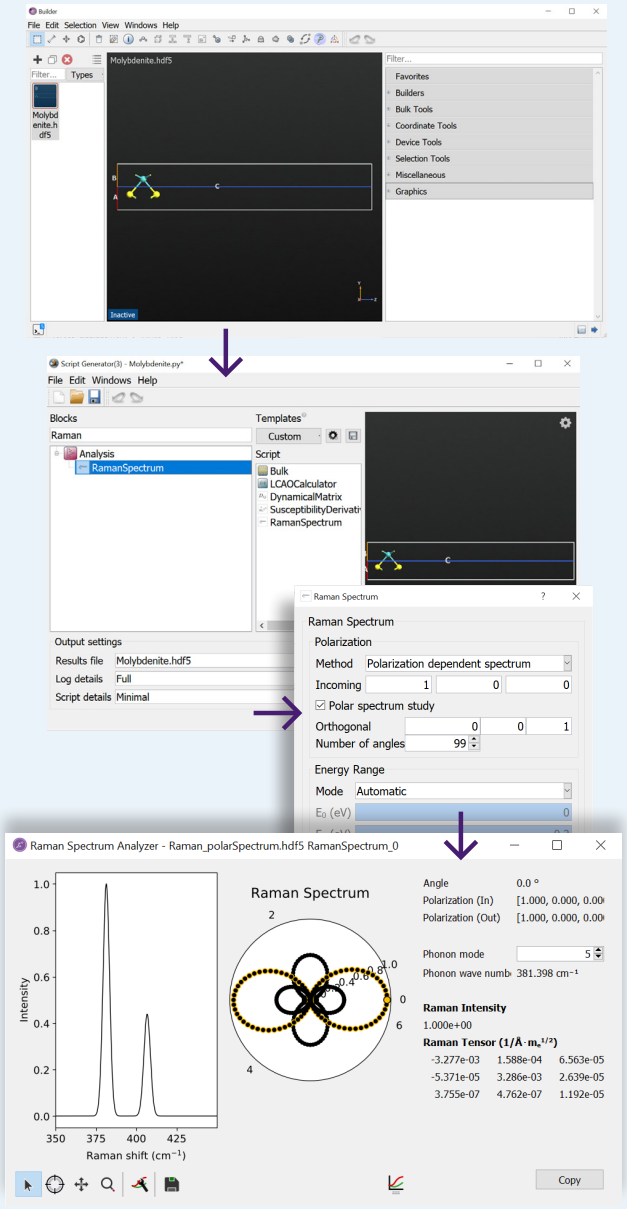
Advanced Analysis Tools

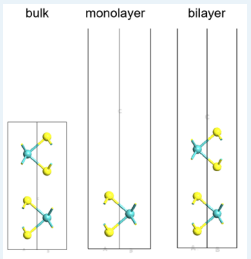
- Use NanoLab GUI analyzers to view, analyze and plot results
- Resolve different phonon contributions to optical properties

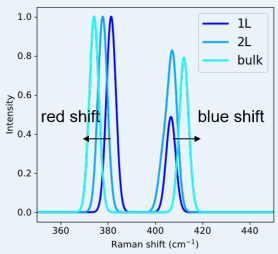
High Performance

- Utilize the full MPI-parallelization of QuantumATK and speed-ups from the symmetry-reduction of wavevector samplings

Case Study: Raman Spectra of Monolayer MoS_2







QuantumATK reproduces the experimentally [1] observed red-shift of E^1_{2g} and the blue shift of A_{1g} with increasing MoS_2 thickness.
[1] Nanoscale, 2014, 6, 5394.

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