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 scripter 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 $E_{1g}$ and the blue shift of $A_{1g}$ with increasing MoS$_2$ thickness.