INDIAN INSTITUTE OF TECHNOLOGY BOMBAY

MATERIALS MANAGEMENT DIVISION

Powai, Mumbai 400076.

Technical Specifications

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Synopsys Quantum ATK with NEGF for Nanomaterial/Nano Devices Simulation

Sr. No	Item Description	Detailed Technical Specification	Technical Compliance (Yes / No)	Additional Information (if any)
1	Synopsys Quantum ATK with NEGF for Nanomaterial/Nano Devices Simulation Quantum-mechanical computational methods.	LCAO-based Density Functional Theory (DFT). Numerical atomic orbital basis sets (SIESTA type) Inclusion of indirect atom pairs for improved accuracy Norm-conserving Troullier-Martins pseudopotentials FHI/HGH/OMX/SG15 potentials provided for almost all elements of the periodic table, including semi-core potentials for many elements. OMX and SG15 potentials are fully relativistic DFT+1/2 method. Ghost atoms (vacuum basis sets) for higher accuracy in the description of surface and vacancies. Virtual crystal approximation (VCA) Introduction of LocalTB09 MGGA functional for better band gap predictions at reduced computational cost.		

		Implementation of Finite Difference Linear Response (FDLR) for ab initio U calculations. Faster and more accurate dispersion corrections with D3 methods. Improvements in project management, amorphous structure generation, array job support, and new analysis tools like thermoelectric coefficients and combined GIF/movie export. Plane wave DFT method. HSE06 exchange-correlation functional. Semi-empirical tight binding Extended Hückel Calculator. Slater-Koster Calculator. DFTB-type model. 30 different parameter sets are shipped with the product, and more can be downloaded and used directly. Built-in Slater-Koster models for group IV and III-V semiconductors. Extended Hückel model with over 300 basis sets for (almost) every element in the periodic table. Spin-orbit interaction (parameterized). Flexible and customizable verbosity framework to control the level of output to the log files		
2	Classical empirical potentials.	Force Field. Over 280 bond-order potentials included. Two/three-body potentials: Lennard-Jones (various versions), Coulomb (various versions), Stillinger-Weber, Tersoff (various versions), Brenner, Morse, Buckingham, Vessal, Tosi-Fumi, user-defined tabulated. Many-body: EAM, MEAM, Finnis-Sinclair, Sutton-Chen, charge-optimized many-body (COMB). Support for custom combinations of potentials. Parallelized via OpenMP for optimal multicore performance (MPI parallelization in implementation).		
3	Electrostatic models	Solvate molecules, slabs, or one-probe surfaces, and perform geometry optimization and transition state search with DFT-LCAO		

		Compute polarization charges, solvation energies, and wettability/surface wetting, contact angle from Young's law COSMO-RS module and GUI analyzer to obtain thermodynamic properties of liquids Built-in database for 1500 molecules Compute acidity (pKa), gas and solid solubility, partition coefficient, vapor pressure, liquid mixture (LLE), sigma plot Support for charged systems.		
4	NEGF method for two-probe systems.	Non-equilibrium Green's function (NEGF) description of the electron distribution in the scattering region, with self-energy coupling to two semi-infinite leads (source/drain electrodes). Open boundary conditions (Dirichlet/Dirichlet) allow application of finite bias between source and drain for calculation of I-V curve. Includes all spill-in contributions for density and matrix elements. Use of electronic free energy instead of total energy, as appropriate for open systems. Ability to treat two-probe systems with different electrodes (enables studies of single interfaces like metal-semiconductor or p-n junctions, for instance). Ability to add electrostatic gates for transistor characteristics (see above under "Electrostatic models"). Improved simulation accuracy for gated devices using Neumann boundary conditions and a new non-uniform grid Poisson solver. Enhanced inelastic transmission spectrum (IETS) analysis and thermal displacement approximation.		
5	Supports GPU acceleration with the DFT, Semi-Empirical, NEGF and Ion dynamics for the large-scale simulations (100,000 atoms).	NA		
6	Surface Green's function method for single surfaces.	NEGF description of the surface layers, with self-energy coupling to a semi-infinite substrate (replaces the slab approximation with a more physically correct description of surfaces). Appropriate boundary conditions for infinite substrate and infinite vacuum above the surface, both for zero and finite applied bias on the surface.		

		Expanded defect simulation capabilities, including new blocks for analyzing defects across interfaces and RSSE for single defects in infinite crystals. Enhanced surface process simulation tools, with a focus on deposition, etching, and advanced thermochemical selectivity analysis.		
7	Performance and stability options.	Scattering states method for fast contour integration in non-equilibrium (finite bias). O(N) Green's function calculation and sparse matrix description of central region. Double or single semi-circle contour integration for maximum stability at finite bias. Ozaki contour integration to capture deep states. Sparse self-energy methods to save memory. Options to store self-energies to disk, either during calculation (instead of RAM) or permanently, to reuse in other calculations. Adaptive (non-regular) k-point integration for transmission coefficients. Addition of methods for thermodynamic integration, quasi-harmonic free energy optimization, and semi-grand canonical Monte Carlo simulations.		
8	Calculation of I-V curves.	Elastic, coherent tunneling transport Quasi-inelastic (LOE) and fully inelastic (XLOE) electron-phonon scattering. Works with any combination of methods for the electronic and ionic degrees of freedom (DFT, tight-binding, DFTB, classical potentials). Many performance options, such as averaging over phonon modes (bunching), using energy-dependent relaxation energies, and repeating the density matrix for homogeneous systems. Inelastic transmission spectrum (IETS) analysis. Special thermal displacement (STD) approximation to efficiently capture the effect of phonon scattering on the I-V curve by creating a canonical average over all phonon modes.		
9	Deep-level analysis of transport mechanisms	Transmission coefficients (k-point/energy resolved) Monkhorst-Pack or edge-to-edge zone filling k-point scheme, or sample only part of the Brillouin zone for detailed information | updated in 2016 Spectral current Transmission spectrum, eigenvalues, and eigenchannels		

		Device density of states, also projected on atoms and angular momenta Voltage drop. Molecular projected self-consistent Hamiltonian (MPSH) eigenvalues Current density and transmission pathways Spin-torque transfer (STT) for collinear/non-collinear spin Atomic-scale band diagram analysis via LDOS or device DOS		
10	Transport properties of fully periodic systems.	Complex band structure. Bulk transmission spectrum.		
11	Machine-Learned (ML) Force Fields | Moment Tensor Potentials (MTPs)	100-1000x faster generation of realistic structures of complex multi-element crystalline, amorphous materials & interfaces, defect and dopant migration barriers, thermal transport, crystallization vs. DFT. Systematically improvable MTPs Active learning MTP simulations to automatically add DFT training data during molecular dynamics (MD) simulations. Employ provided MTP potentials for Si or develop potentials for new materials and problems using automated training and simulation workflows Enhanced performance and memory optimization for M3GNet, enabling larger molecular dynamics simulations (up to 30,000 atoms). Faster MTP training (10–15x) and new optimization techniques, such as Particle-Swarm Optimization for nonlinear parameters. Expanded functionality of M3GNet and MACE-MP for simulating devices, slabs, and molecules.		
12	Complex Semiconductor Materials, Interfaces & Gate Stacks	Use ML MTPs for obtaining realistic crystalline, amorphous materials, interface, gate stack structures, simulating dopant diffusion, thermal transport, and crystallization Plot band edges in projected DOS, local DOS and projected local density of states analysers. Defect and dopant simulation improvements.		
13	1D & 2D-Material Based FETs.	More accurate band diagrams and device I-V characteristics with the new HSE06-NEGF methodology compared to PBE-NEGF. More accurate on-state calculations using Neumann boundary conditions in the transport		

		direction compared to Dirichlet at the Semi-Empirical level. Up to 80% faster simulations of gated devices with vacuum regions using the new Poisson solver using a non-uniform grid compared to the parallel conjugate gradient (PCG) solver.		
14	Advanced Surface Process Simulations.	Enhanced surface process simulation module enabling scanning over a range of impact energies and incident angles of “shooting” atoms at a surface for maximum yield in sputtering, etching (ALE) and deposition (ALD) processes. Use the newly implemented thermochemical selectivity analysis tools in the GUI to screen critical reactions in a process, find ideal reactants and optimal reaction conditions for the processes. Compute quantities, such as sputtering yield and sticking coefficient, needed for feature scale and reactor scale models.		
15	Platform & Infrastructure	QuantumATK is delivered as a self-contained binary installer, with no compilation needed and no external library dependencies beyond standard operating system packages. Runs on all modern 64-bit Windows and Linux versions High-performance OpenGL shader-based rendering engine for very large data sets (1M+ atoms) on both Windows and Linux: Fall-back protocol to simpler models for low-end graphics hardware, including software rendering if necessary Provides a complete Python3 environment Includes precompiled optimized libraries like numpy/scipy/ScaLAPACK (based on MKL), sympy, pandas, matplotlib/pylab, MPI4Py, SSL bindings, sklearn, pytorch, pymatgen, ASE, fireworks, Qt/PyQt, and many more Supports pip for installation of additional Python modules, either in main installation or through virtual environments All output data stored in HDF5 files Add-on manager for installing plugins from Synopsys or third-party developers		
16	Warranty of the system	1 year		

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