Victory Atomistic

Nanostructure Material and Quantum Device Simulator

Below ten nanometers, designing the most advanced technological architectures requires simulations at the atomic scale. Silvaco and the Purdue Research Foundation have teamed up to create an atomistic simulation solution for next-generation semiconductor devices and materials called Victory Atomistic.

Thanks to Victory Atomistic's combination of non-equilibrium Green's functions (NEGF) and state-of-the-art band structure calculations, versatile, predictive, and fast simulations become easy to perform, even without full academic knowledge of the NEGF theory; the complexity is hidden inside the simulation tool, which benefits from years of development at the highest level.

Nanotechnology products exhibit advanced quantum physical effects. The engineering of nanoelectronics aims to optimize a myriad of constraints in these domains: non-uniformities, strains, confinements, tunnel effects, and thermal, optical, and magnetic responses. Victory Atomistic addresses these constraints in its comprehensive analysis.

Victory Atomistic optimal solution allows users to obtain a meaningful I(V) curve daily on a conventional computer. Its integration within the Silvaco environment provides an atomistic set-up and visualization framework, allowing a smooth transition toward emerging materials and technologies for TCAD users.

Key Features of Victory Atomistic

- Device simulator functional at atomic resolution for 2D and 3D materials
- Integrated into Silvaco's TCAD DeckBuild environment
- Advanced visualization with companion tool VictoryVisual
- Multiple physics solvers
    - Self-consistent Poisson-Schrödinger
    - Force-field relaxation, strain-dependent calculation
    - Quantum Transmission Boundary Method (QTBM)
    - Non-Equilibrium Green's Function (NEGF)
    - Electron-phonon and phonon-phonon self-energies
    - Mode-space and low-rank approximation compatible with scattering
    - Büttiker-probes method
- Electronic structure calculations: band-structure, density of states, transmission probability
- Atomic prediction of potentials, charges, mobilities, and band edge shifts that can serve as input to traditional TCAD
- Device simulation of MOSFET, TFET, and LED, thanks to device templates and meta-solvers
- I(V) characteristics, density of states, and current density resolved in space and energy
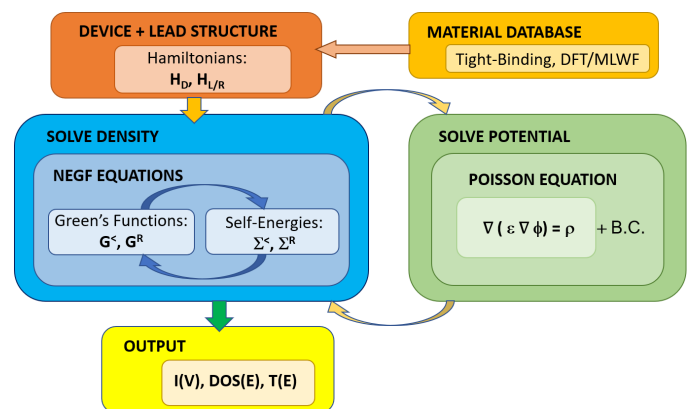- Amazon cloud-ready, parallel MPI/OpenMP runs in batch mode.

Nanoelectronics

Victory Atomistic can solve for various architectures with atomic resolution thanks to an ingenious device builder fed by a material database containing an advanced set of tight-binding parameters that the user can also enrich with forefront ab initio results.
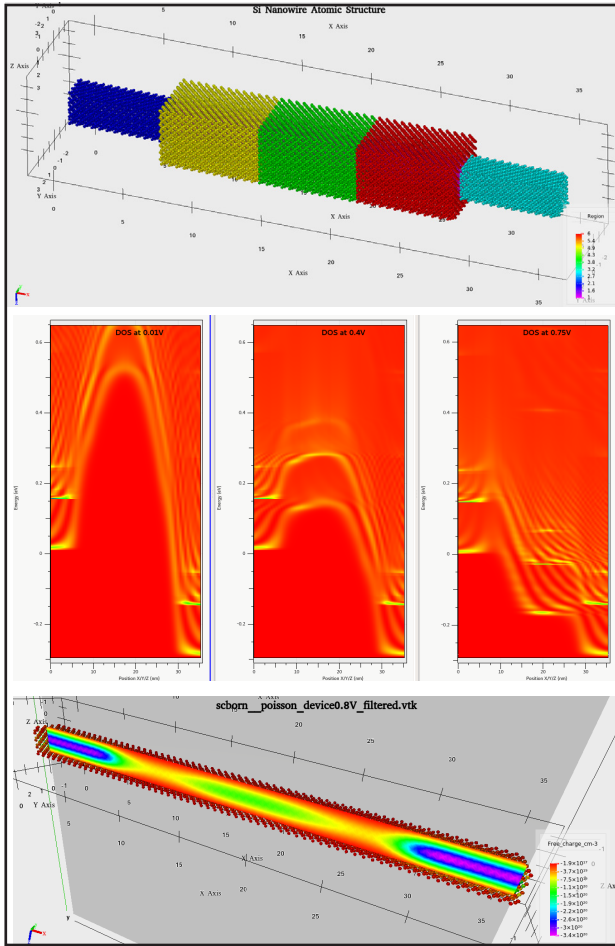
The Victory Atomistic goes far beyond ballistic approximations to treat essential coherent and incoherent scattering mechanisms, thanks to NEGF. At the heart of the simulator, the computational burden of self-energies is drastically reduced, thanks to low-rank approximation techniques that preserve numerical accuracy.


Victory Atomistic Flowchart of Atomistic Solvers

A silicon nanowire FET with 20 orbitals per atom and 8 000 atoms with modespace and electron-phonon scattering: visualization of the NEGF results with Victory Visual
Top: NWFET structure with spacers
Middle: Density of States resolved in space and energy for different grid voltages
Bottom: Free charges in the NWFET
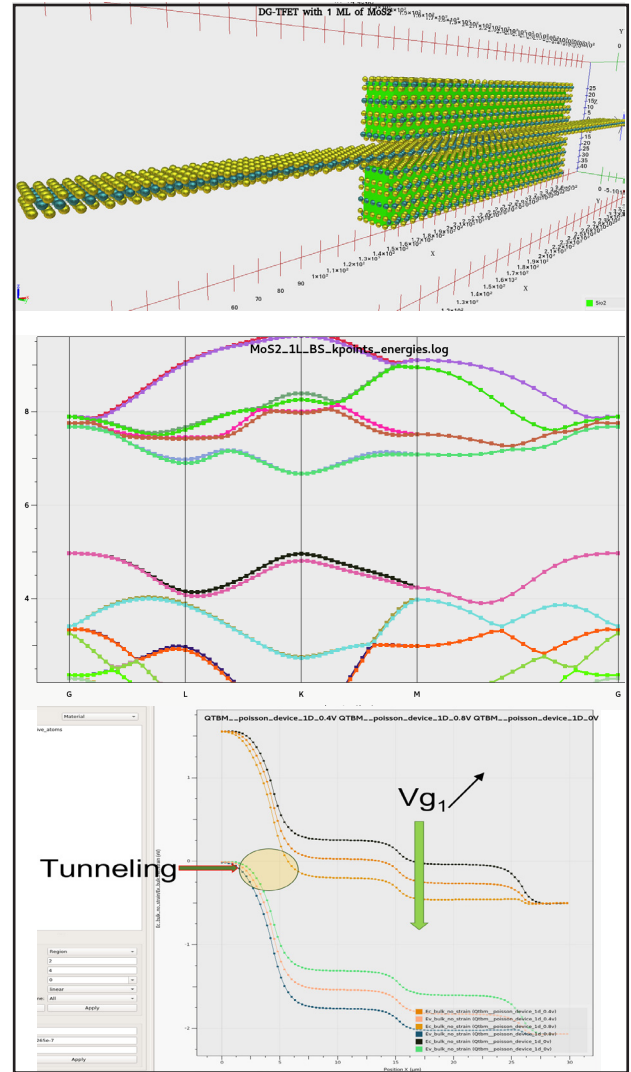
Dual-gate TFET with one monolayer of MoS2 – Top: device structure with insulator (green), Mo (blue) and S (yellow) atoms
Middle: Band Structure of the Wannier Hamiltonian
Bottom: TFET 1D band profile function of the gate voltage applied
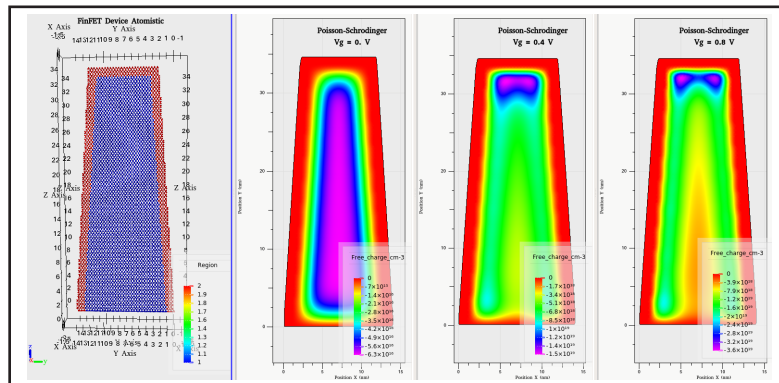
FinFET Q(V) calculation using Poisson-Schrödinger atomistic solver
Left: Finfet structure – followed by the charge with increasing gate voltage