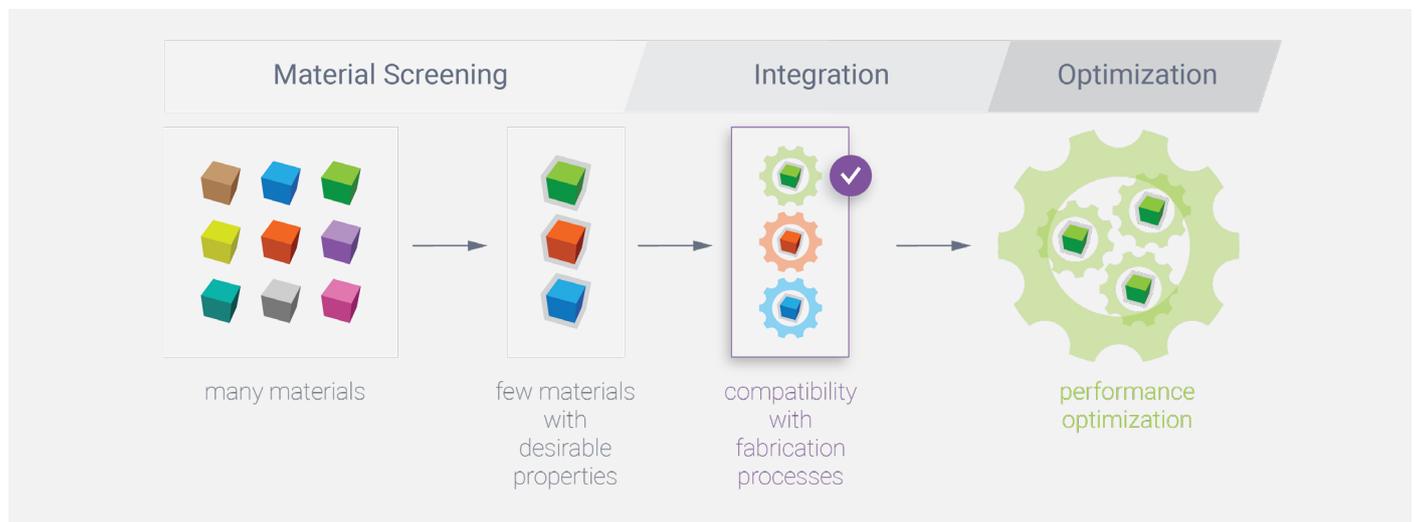
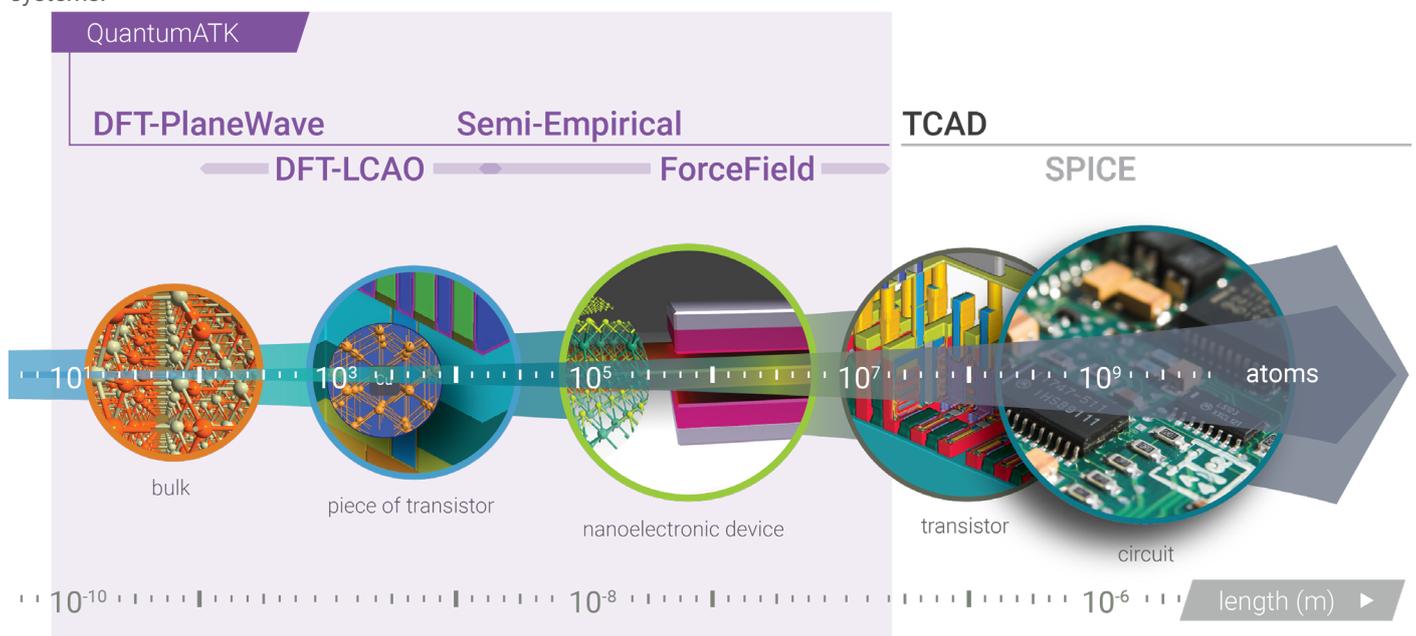


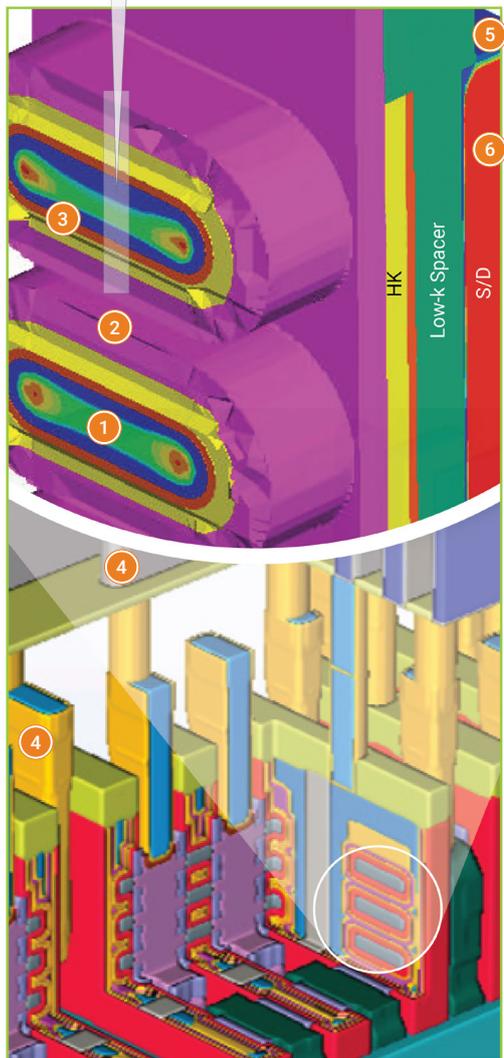
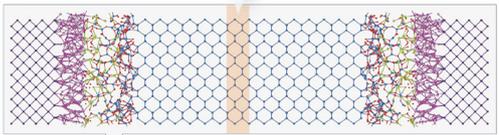
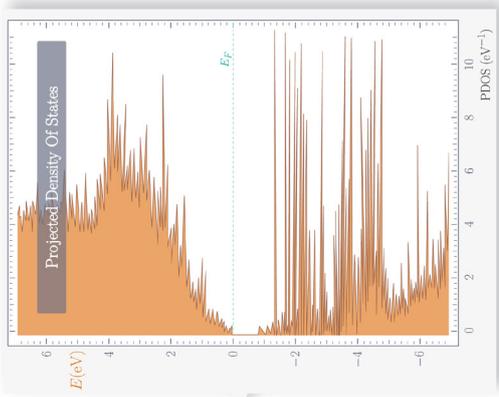
QuantumATK Software Solution for Advanced Semiconductor Development

The exponential growth in computer power in combination with new advancements in algorithms has in recent years enabled the practical application of atomic-scale modeling to the R&D of new materials and product design across a broad range of high tech industries. A key benefit of atomistic modeling is the detailed insight into the atomic-scale processes which complement experimental data and make the R&D process more efficient through higher quality end results and cost-effective and faster downselection of material options (materials screening).



QuantumATK is a complete atomistic simulation toolkit developed and supported by world leading atomic-scale modeling experts. QuantumATK reduces time and cost in advanced semiconductor technology development by enabling earlier co-optimization of materials processes and transistors. The integration of QuantumATK with Sentaurus TCAD provides a seamless flow from material to device (as shown in the picture below). Atomic-scale modeling tools in QuantumATK range from classical force fields for handling large and to some extent more realistic materials systems to ab initio tools that provide highly accurate results for smaller systems.



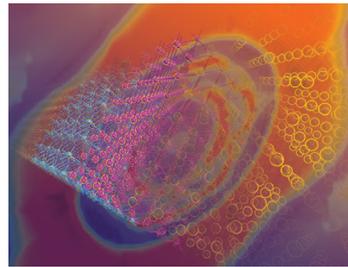


- ① Channel Materials in Nanoscale Geometries
- ② Workfunction Engineering
- ③ Surface Scattering
- ④ Alternative Interconnect Metals
- ⑤ Contact Resistance
- ⑥ Dopant Diffusion/Activation in S/D

QuantumATK addresses key applications in the semiconductor industry and is a core component of the Synopsys Design-Technology Co-Optimization flow. QuantumATK offers modeling solutions for critical materials issues in advanced semiconductor technology development:

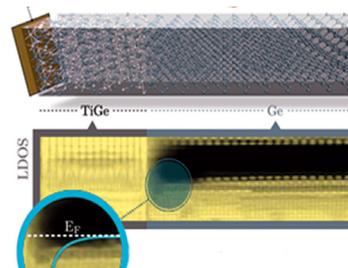
- Exploration of alternative interconnect metals
- Modeling and optimization of metal-semiconductor contacts
- Bandstructure and carrier transport modeling in new channel materials within quantized transistor structures
- Exploration and optimization of high-k dielectric and ferroelectric stacks
- Mechanical modeling of collapse of fins and pillars
- And many other critical issues

Highlighted Publications with QuantumATK



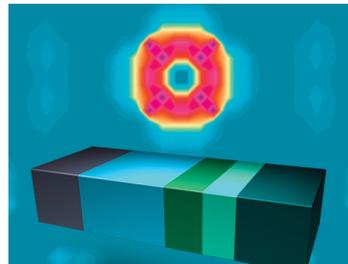
Electron Scattering at Interfaces in Nanoscale Vertical Interconnects: A Combined Experimental and Ab-Initio Study

Study by IBM & GlobalFoundries | Lanzillo et al., Appl. Phys. Lett. 112, 163107 (2018)



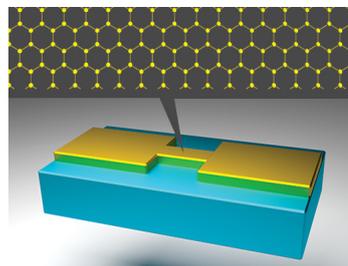
First-Principles Investigations of TiGe|Ge Interface and Recipes to Reduce the Contact Resistance

Study by GlobalFoundries & IBM Research | Dixit et al., IEEE Trans. Elec. Dev. 64, 3775 (2017)



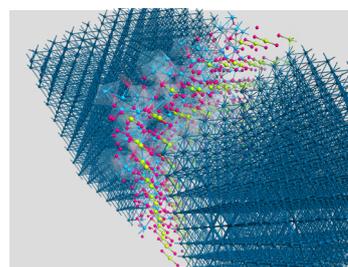
Oscillatory Behavior of the Tunnel Magnetoresistance Due to Thickness Variations in Ta|CoFe|MgO Magnetic Tunnel Junctions

Study by Imec, PLASMANT and Synopsys QuantumATK Team | Sankaran et al., Phys. Rev. B 94, 094424 (2016)



Theoretical Study on High Frequency Graphene|Nanoribbon Heterojunction Backward Diode

Study by Fujitsu Ltd. and Fujitsu Laboratories Ltd. | Harada et al., Appl. Phys. Expr. 10, 074001 (2017)

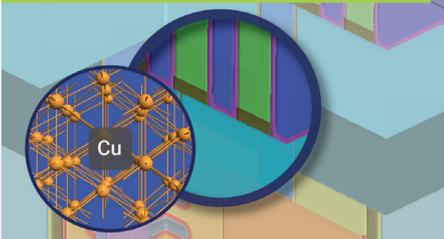


Electron Transport Across Cu|Ta(O)|Ru(O)|Cu Interfaces in Advanced Vertical Interconnects

Study by IBM Research at Albany Nanotech and IBM T.J. Watson Research Center | Lanzillo et al., Comp. Mat. Sci. 158, 398 (2019)

Highlighted QuantumATK Applications

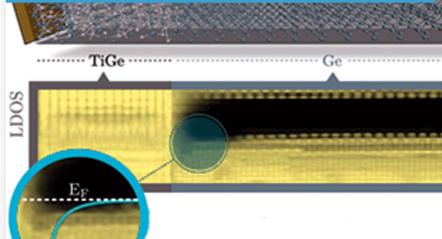
Interconnects



Explore Alternative Interconnect Metals

- Support the screening and characterization of metal alternatives to Cu and barrier materials
- Calculate the mean free path and resistivity in metals and alloys and evaluate the impact of surface and grain boundary scattering
- Optimize the composition and thickness of diffusion barriers
- Calculate the resistance of the interface between interconnect and barrier metals

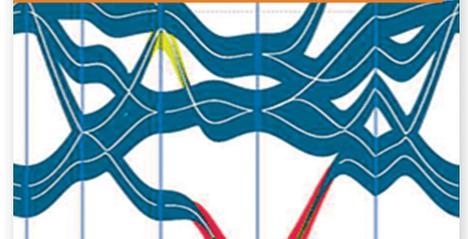
Metal-Semiconductor Contacts



Optimize Metal-Semiconductor Contacts

- Investigate how the atomic structure of the interface impacts the contact resistance
- Determine the intrinsic processes that limit the contact resistance
- Obtain doping-dependence of contact resistance
- Simulate band alignment and offset at interfaces
- Calculate Schottky barriers

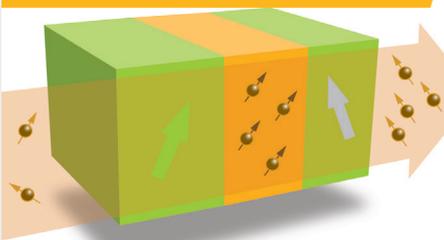
Transistor Channels



Model Bandstructure and Carrier Transport

- Calculate bandstructures and extract band parameters to be inserted in TCAD advanced transport simulations
- Obtain phonon-limited electron-mobility
- Generate random alloys for any type of geometry using our builtin genetic Special Quasi-Random Structures (SQS) algorithm

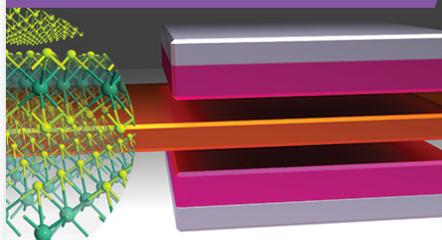
Spintronic Memory



Optimize Material Stacks for Spintronic Memory

- Investigate and optimize material stacks comprising the magnetic tunnel junctions (MTJ) in the STT-RAM bit cells
- Calculate tunnel magnetoresistance ratio (TMR)
- Simulate spin-polarized tunneling current
- Determine bias-dependent spin-transfer torque based on non-collinear spin NEGF transport
- Simulate non-ideal material stacks, such as oxidized interfaces and impure materials

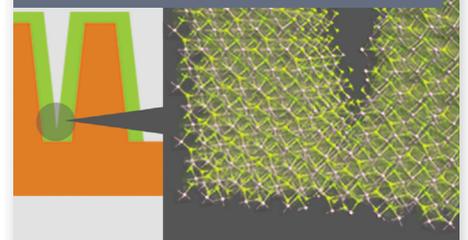
Nanoelectronic Devices



Simulate Nanoelectronic Devices

- Perform electronic and thermal-transport analysis
- Obtain current-voltage characteristics (I-V curve)
- Calculate leakage current
- Include electron-phonon scattering effects (EPCs)
- Investigate various architectures

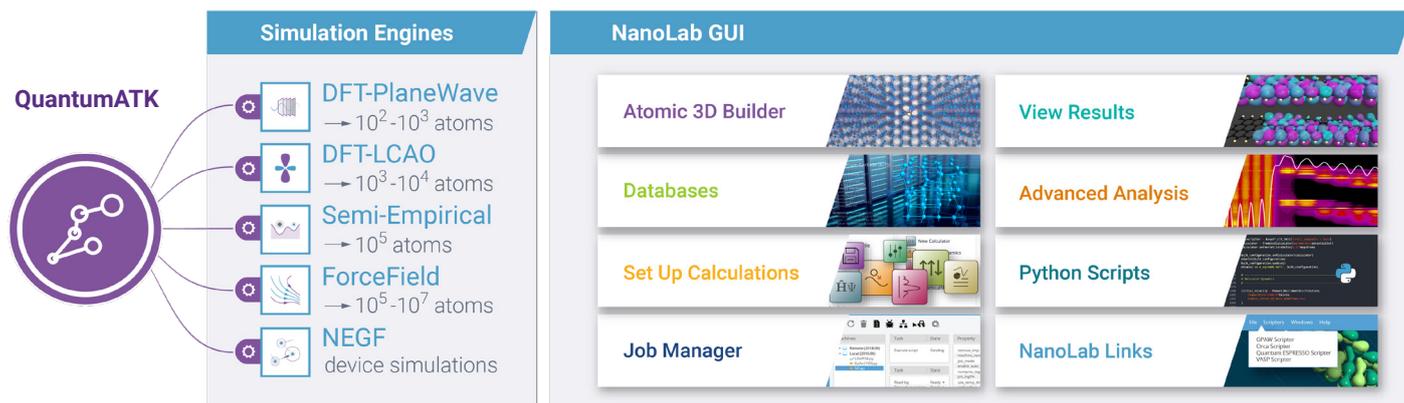
Collapse of Fins and Pillars



Model Collapse of Fins and Pillars

- Get insights into the pattern collapse due to zipping effect that happens during layer deposition on top of fins.
- Extract the bonding force per unit area and plug it into transistor scale analysis in Sentaurus Interconnect.
- Improve manufacturing yield and avoid pattern collapse by using predictive atomic scale analysis to re-engineer material composition or by re-engineering process conditions

QuantumATK is a complete and fully integrated software suite for atomic-scale modeling of semiconductors, professionally engineered using state-of-the-art scientific and software-engineering methods. It combines the power of a Python scripting engine with the ease-of-use provided by an intuitive graphical user interface. All simulation engines share a common infrastructure for analysis, ion dynamics and parallel performance techniques. The platform consists of the following components:



Calculators

- **DFT-LCAO:** Simulation engine for density functional theory (DFT) using pseudo-potentials and linear combinations of atomic orbitals (LCAO) basis sets.
- **DFT-PlaneWave:** Simulation engine for DFT using pseudo-potentials and plane-wave basis sets.
- **SemiEmpirical:** Semi-empirical simulation engine using DFTB, extended Hückel, Slater-Koster, and other tight-binding models.
- **NEGF:** Module for nanoscale device and transport simulations using non-equilibrium Green's function (NEGF) methodology. Uses either DFT-LCAO or the SemiEmpirical module for describing the Hamiltonian of the system.
- **Surface Green's Function:** Module for modelling of surfaces beyond the slab approximation. Allows for treating electro-chemical reactions and surface states. Uses either DFT-LCAO or the SemiEmpirical module for describing the Hamiltonian of the system.
- **ForceField:** Simulation engine for atomic-scale simulations (e.g. molecular dynamics) using classical potentials such as bonded and reactive force fields, pair potentials, and other parameterized interaction models for atoms.

GUI

- **NanoLab:** Graphical user interface (GUI) for all QuantumATK calculators.
- **NanoLab Links:** Module enabling NanoLab to interface other codes.

Scripting and Parallelization

- **Python Scripting and Automatization:** Component that binds the DFT, Semi-empirical and force field calculators together in a common interface and allows them to synergistically work together. It enables users to automate and customize tasks (also in NanoLab).
- **Distributed Processing:** Common module for all QuantumATK calculators which enables MPI parallelization and distributed memory, in order to split the computational workload over a number of computing nodes (CPUs) to reduce turn-around-time (TAT).
- **Threaded Processing:** All QuantumATK calculators allows for parallel computing using threading on shared memory systems. Threading can be combined with MPI to thread on multi-core compute nodes and connect many nodes using MPI.

Common Modules

- **Ion dynamics:** NVT, NPT, NVE ensembles with a range of different thermostats and barostats. Geometry and reaction path optimization (NEB) with Quasi-Newton and Fire methods. Flexible geometry constraints and a rich collection of analysis methods. Works seamlessly with the DFT, SemiEmpirical and ForceField calculators.
- **Electron-Phonon interaction:** Compute deformation potentials and conductivity/mobility tensor via the Boltzmann equation. Extract Hall coefficient and Hall conductivity tensor, Seebeck coefficient and ZT. Available with the DFT-LCAO and SemiEmpirical calculators.
- **Poisson Solvers:** Insert gates, dielectric regions or implicit solvent models in devices or periodic structures. Use of periodic, Dirichlet, Neumann or multipole boundary conditions. Supported by the DFT and SemiEmpirical calculators.
- **Property Calculations:** Extensive list of methods for calculation of mechanical, electronic, magnetic, electrical and optical properties.



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