

QuantumATK for Advanced TCAD

Modeling semiconductor material
properties and device characteristics
at the atomic scale

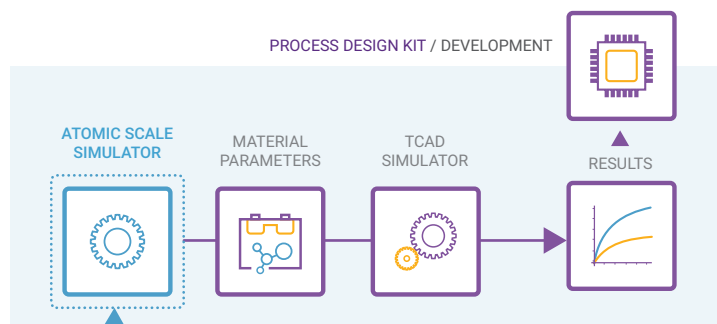
Use **QuantumATK** to model properties of semiconductor materials and nanostructures and study ultra-scaled device characteristics and performance.

Advantages of QuantumATK

- Industry proven
- [Market leading software package for device simulations](#)
- Becoming integrated with Sentaurus TCAD and TCAD-to-SPICE through the newly released Sentaurus Materials Workbench: investigate the impact of semiconductor materials choices at the circuit level
- [One software package for computing electronic, electric, thermal, optical and mechanical properties](#)
- Advanced Graphical User Interface for the full research workflow
- [Customized tools, support and training](#)

Benefits of Atomic-Scale Modeling

- Stay ahead through improved/increased product/technology design and cutting-edge innovation
- [Achieve the target performance and power of new technology nodes as semiconductor technology continues to scale](#)
- Reduce costs (save time and money) by minimizing the need of expensive and time-consuming experimental prototyping and testing and lower barriers to innovative ideas



RESEARCH
DEVELOPMENT
INTEGRATION
PRODUCTION

QuantumATK Leading industry-proven atomic-scale modeling software

- **Quantum:**
First principles Density Functional Theory (DFT) for parameter free simulations (~5000 atoms) and Semi-empirical methods (~105 atoms).
- **ForceField:**
Simulations with more than 300 built-in classical potentials (~106 -107 atoms).
- **NEGF:**
Model nano-scale devices and their characteristics and surfaces with the Non-Equilibrium Green's Function (NEGF) method.
- **NanoLab/NanoLab-Links:**
Advanced GUI for Quantum, Force Field, NEGF and external simulation engines like VASP, Quantum ESPRESSO and LAMMPS.

Since 2006, over 1200 scientific articles have been published using QuantumATK.
The software is used by over 300 research groups at leading universities, labs, and in the electronics industry around the world.

Electronic and Mechanical Properties

- Thermoelectrics (Bi₂Te₃, etc.)
- High-k dielectrics (HfO₂, etc.)
- IV materials (GeSn, SiGe, etc.)
- III-V materials (GaN, hBN, etc.)
- 2D materials (graphene, silicene, etc.)
- Metallic alloys

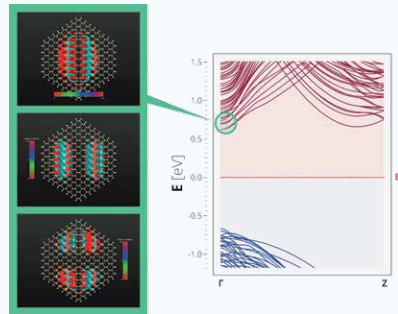


Figure 1:
Band structure
of a Si nanowire

Dynamic Processes

- Ion/defect diffusion
- Diffusion length
- Activation barriers
- Aging
- Growth

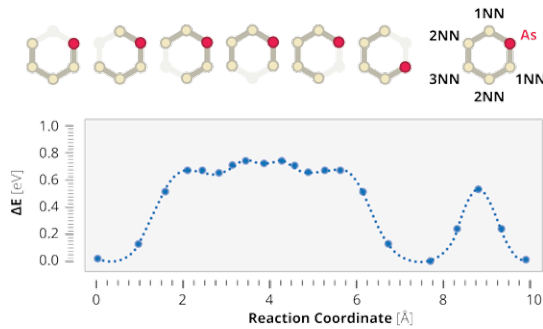


Figure 2:
Study by Global Foundries
and Synopsys on As-vacancy
pair diffusion in Si.
Y. Park *et al.*, IEDM (2017)

Interfaces Between Materials

- Metal-semiconductor interfaces
- Grain boundaries
- Contact resistance
- Schottky barriers
- Doping

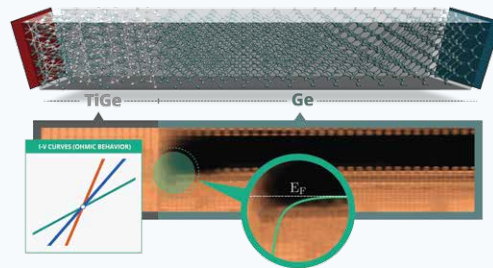
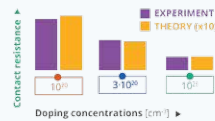


Figure 3:
Study by Global Foundries
and IBM Research on the
TiGe/Ge contact
resistance

H. Dixit *et al.*,
IEEE Trans. on
Elec. Dev. 64,
3775 (2017)

Emerging Nano-Devices

- Transmission functions
- Current-voltage characteristics
- Thermal transport
- Leakage current
- Electron-phonon scattering effects
- Architectures: MOSFETs, FinFETs, TFETs, vertical/horizontal nanowires, nanosheets, nanotubes, etc.

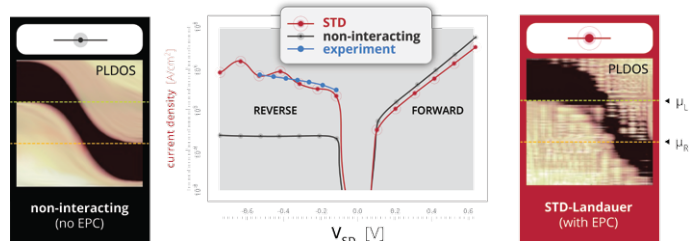


Figure 4: Si p-n junction. T. Gunst *et al.* Phys. Rev. B 96, 161404 (2017)

Spintronic Devices

- Magnetoresistance
- Interfacial resistance at the junction
- Spin transfer torque
- MRAM and STT-MRAM
- Topological insulators

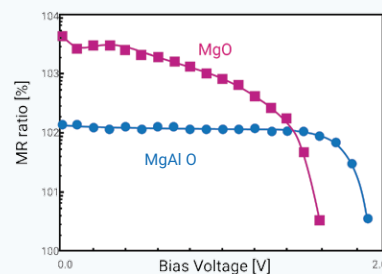


Figure 5:
Magnetoresistance in
Fe/MgAl₂O₄/Fe and
Fe/MgO/Fe junctions

Masuda *et al.*,
Phys. Rev. B 96,
054428 (2017)



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