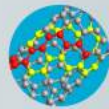
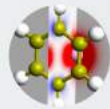
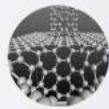
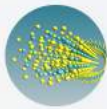


ATOMISTIX TOOLKIT

Atomic-Scale Modeling Software for Nanotechnology

Atomistix ToolKit (ATK) offers unique capabilities for simulating electrical transport properties of nanodevices on the atomic scale. Based on an open architecture which integrates a powerful scripting language with a graphical user interface, ATK is a comprehensive platform for studies in nanoelectronics, using both accurate first-principles (DFT) and fast semi-empirical methods and classical potentials. Moreover, ATK includes a very advanced electrostatic model to allow realistic simulations of nanoscale transistor structures.



Study

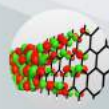
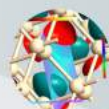
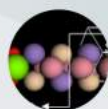
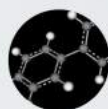
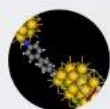
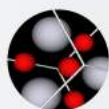
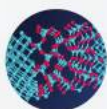
- graphene & nanotubes
- nanowires
- magnetic tunnel junctions
- molecular electronics
- complex interfaces
- high-K dielectrics
- spintronics
- single-electron transistor
- phonons and phonon transport
- transistor DOS
- Nudged Elastic Band
- stress and strain
- topological insulators



ATK

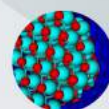
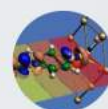
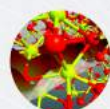
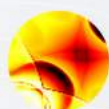
Calculate

- I-V curve
- transistor characteristics
- spin current
- Schottky barrier
- leakage current
- contact resistance
- tunnel magneto-resistance
- charge stability diagram
- classical potential
- Molecular Dynamics nanotube
- complex bandstructure
- transition states
- thermal transport
- spin transfer torque



ATK is also an **ideal tool for educational courses** in various subjects, from basic quantum mechanics to graduate courses in nanoelectronics. Special discounts are available for teaching licenses.

Since 2006, over 800 scientific articles have been published using ATK. The software is used by over 300 research groups at leading universities, government labs, and electronics companies around the world, in a wide range of application areas (see other side).



Download a free trial:

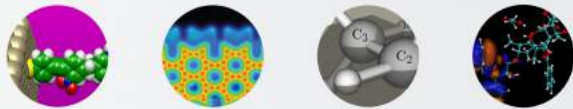
www.quantumwise.com

Application areas

The unique capabilities of Atomistix ToolKit are currently being applied in a wide variety of areas, such as carbon and molecular electronics, nanowires, and spintronics devices, as well as for assessing the structural and electrical properties of new electronic materials like high-k dielectrics or organic electronic materials.

Molecular Electronics

- Current-voltage (I-V) characteristics of rectifying molecular junctions (single molecules between metal electrodes), i.e. molecular diodes and switches. The active component can be an organic or organometallic molecule, a metallic nanocluster, etc.
- Resistivity of insulating or conducting molecular wires, free or attached to surfaces.
- Investigation of optical switches
- Inelastic spectroscopy.



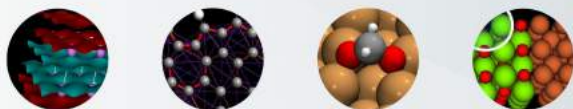
Bulk and nanoscale semiconductors

- Surface states in semiconducting nanowires.
- Leakage currents in ultra-shallow junctions with high/low-k dielectrics.
- Schottky barriers of complex interfaces.
- Activation energies of defect diffusion.
- Work function of nanostructured surfaces (nanoclusters, wires).
- Binding energies of defects in bulk semiconductors, nanowires, or nanotubes.
- Nonparabolicity parameters.
- Phonon limited mobility.



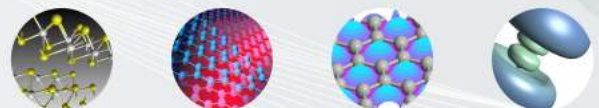
Carbon-based Electronics

- Transport properties (conductance, I-V) of carbon or boron-nitride nanotubes, with or without defects and impurities.
- Graphene nanoribbons, e.g. for field-effect transistor applications; also bilayer structures.
- Multiwall nanotubes, for applications as nanoscale variable resistors or capacitors.
- Contact resistance and capacitance of metal, nanotube and graphene interfaces and junctions.
- I-V characteristics of functionalized nanotubes or graphene for sensor applications.



3-Terminal devices

- Advanced electrostatic model with dielectric and biased metallic region.
- Calculation of transistor characteristics.
- Charge stability diagrams of weakly coupled single-electron transistors in Coulomb blockade regime (sequential tunneling).



Nanowires

- I-V characteristics of metallic nanowires and atomic point contacts.
- Electromigration and non-equilibrium current-induced forces in atomic wires.
- Mobility limited by random scattering.



Magnetic systems and spintronics

- Spin tunneling mechanisms in magnetotunnel junction (MTJ) for MRAM/read applications.
- Spin torque transfer in MTJs.
- I-V characteristics of molecular spintronics structures.
- Non-collinear, including spin spin-orbit.
- Transport properties of magnetic metallic nanowires.



Computational science has become critical to scientific leadership, economic competitiveness, and national security. Breakthroughs and innovations will be won by those most skilled with advanced computing systems and computational science applications.

US President's Information Technology Advisory Committee

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