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ATK: An open platform for atomic-scale modeling

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Atomistix ToolKit (ATK) from QuantumWise is a platform for atomic-scale modeling that provides a user-friendly interface to a wide variety of state-of-the-art simulation codes, including DFT, tight-binding and classical potential methods developed by QuantumWise, as well as external software packages. The platform has a modular structure which allows for development of third-party plugins for extended and customized functionality, a similar concept as the apps known from the iPhone/Android world. This makes the platform extremely versatile and efficient for working on a broad class of nanoscale problems.

ATK is market leader within Quantum Transport simulations. ATK is designed to describe open boundary conditions where the electron density is calculated using NonEquilibrium Green's Function (NEGF) formalism and the electronic structure can be described at the DFT or tight binding level. The electro-statics is described self-consistently through a Poisson multi-grid solver, and allows for electro-static couplings between continuum models and the atomistic models.

For simulation of systems with millions of atoms ATK provides a classical potential package. In the EU project ATOMMODEL with Fraunhofer SCAI, we are developing a new model for on the fly generation of classical potentials from first principles data. The new model will be implemented in the Tremolo-X simulation packages, which will be available from ATK.

QuantumWise profile
QuantumWise specializes in fast and reliable atomic-scale modeling solutions, delivered via an easy-to-use interface. The software package is called Atomistix ToolKit (ATK), and is used by leading academic groups and commercial companies in the areas of materials for electronic devices, catalysis, new emerging electronic devices, graphene materials and other new nanoscale materials.

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