

QuantumATK: Industry-Leading Solutions for Atomic-Scale Modeling Complex Materials, Interfaces, Nanostructures and Electronic Devices

Umberto Martinez & Vaida Arcisauskaite

2-3 March 2021

<https://www.synopsys.com/quantumatk>





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Synopsys Today: From Silicon to Software

 <p>FY20 Revenue: ~\$3.7B</p>	 <p>Employees: ~15,000</p>	 <p>Patents: ~3,300</p>	 <p>Offices: ~125</p>
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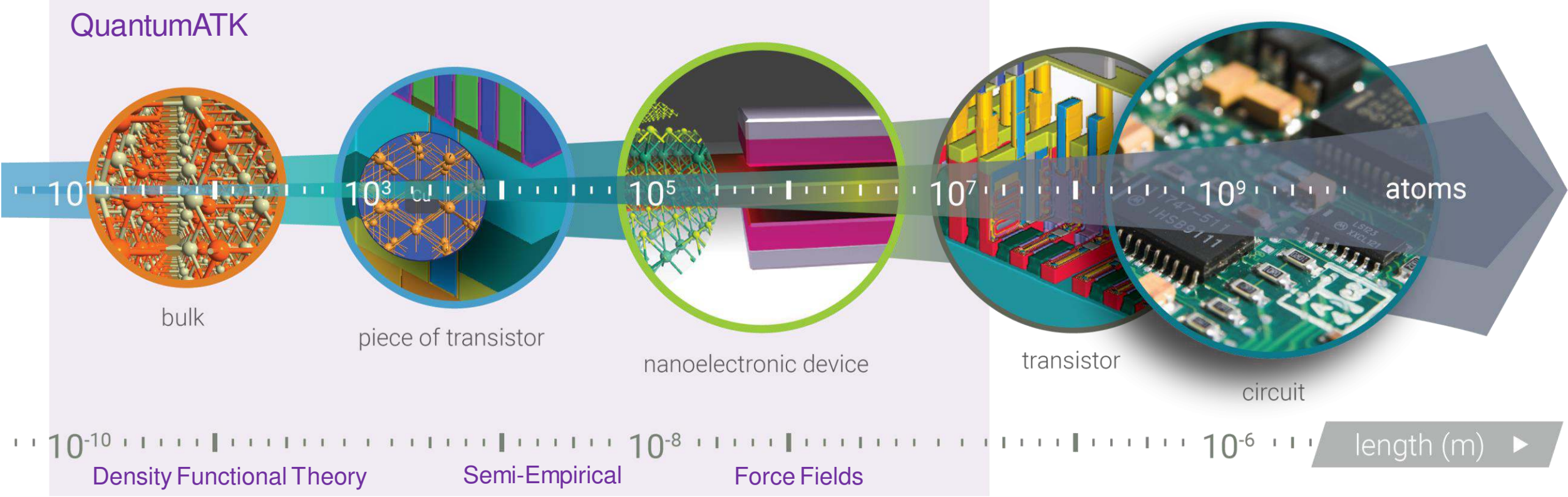


#1 electronic design automation tools & services

Broadest IP portfolio and **#1** interface, analog, embedded memories & physical IP

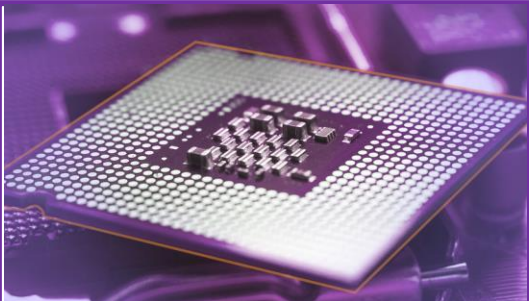
‘Leader’ in Gartner’s Magic Quadrant for application security testing

QuantumATK Multiscale Physics Solutions

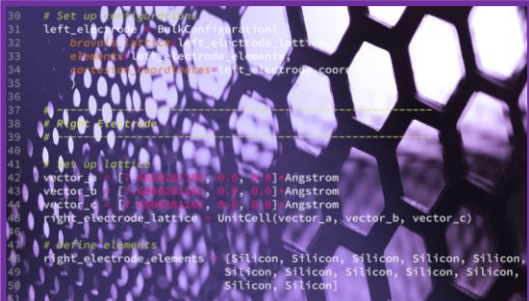


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Atomic-Scale Modeling Benefits



Helps in path finding for solving **current** industrial problems

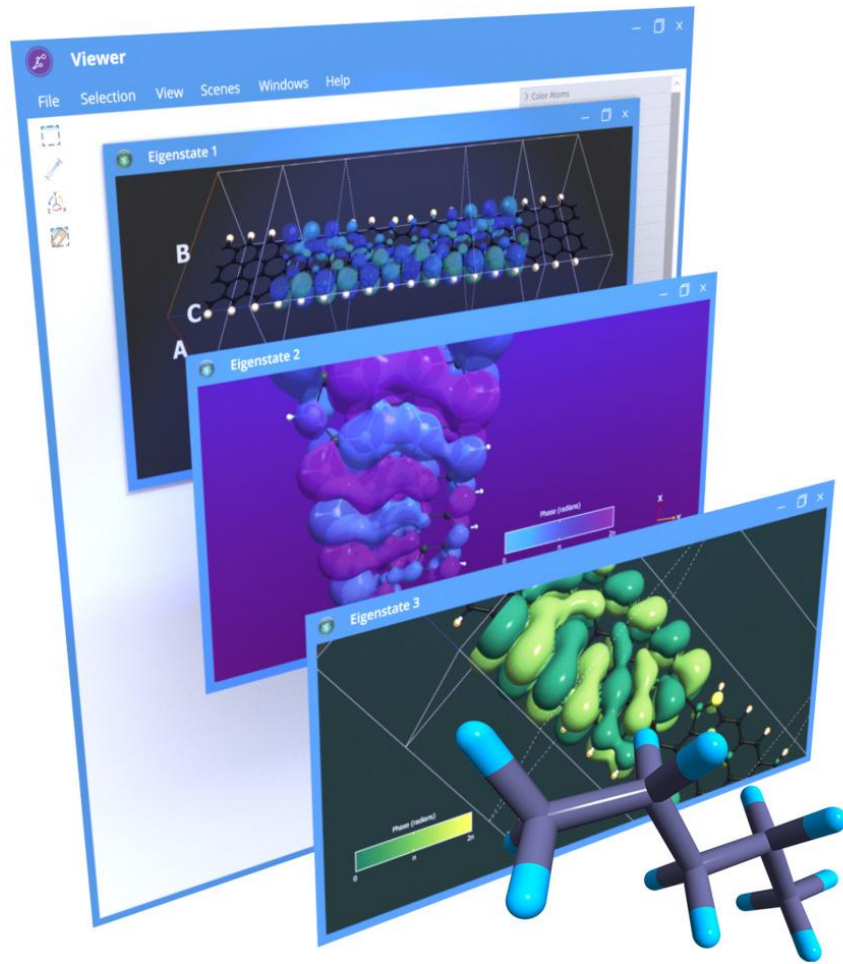


Guides R&D research on **next generation** materials and devices



Reduces R&D time and related costs by running computer simulations instead of experiments

QuantumATK Advantages



1. Effective Tools for All Levels

- ✓ **New Users:** Intuitive interface with quick-and-easy access to all tools and features
- ✓ **Experienced Users:** Power of a Python scripting engine for customization and automation of tasks
- ✓ **Full Support:** Providing customized and novel solutions fast. Expert team of R&D and Application Engineers.

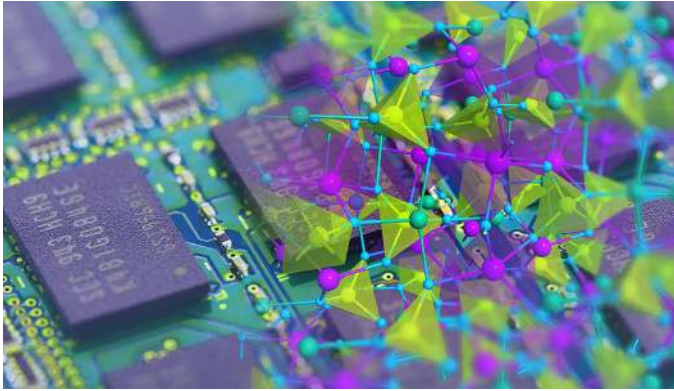
2. Synergistic Solution

- ✓ Multiple simulation methods in **one powerful platform**
- ✓ Integration with **TCAD**

3. Realistic Physics Outcomes in Complex Materials

- ✓ Strong capability to analyze **large scale systems** and thus provide more realistic simulation results
- ✓ Unique features for electron **transport**

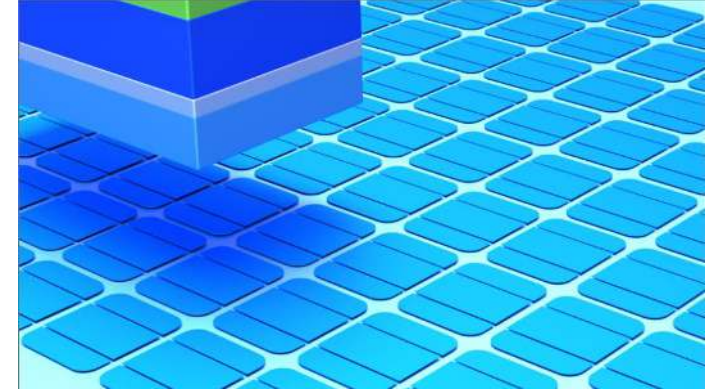
QuantumATK Addresses Key Materials Modeling Areas



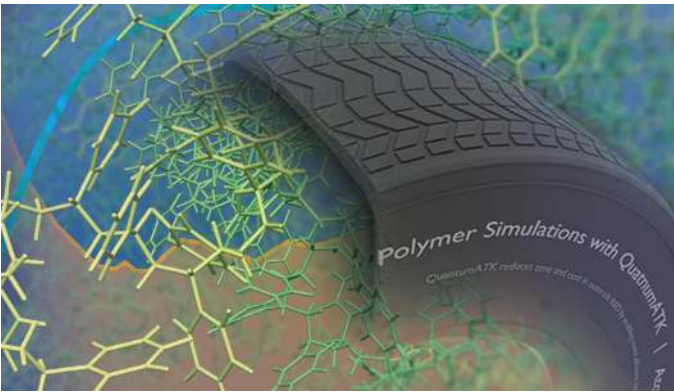
Semiconductors



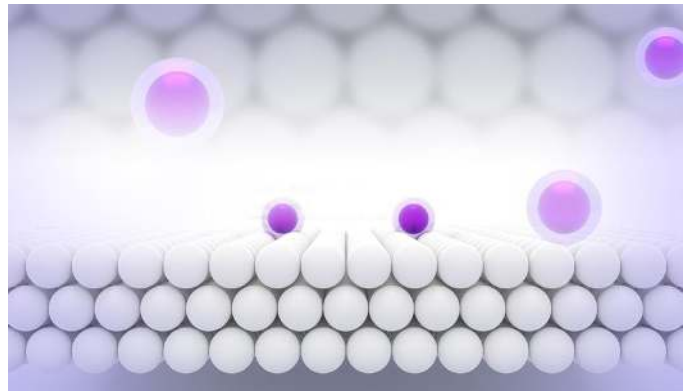
Batteries



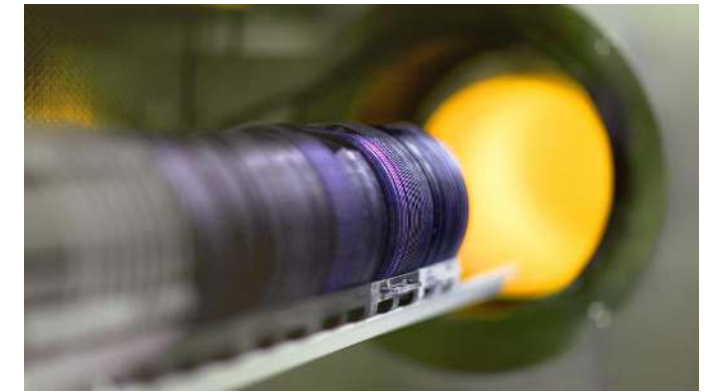
Solar & Fuel Cells



Polymers

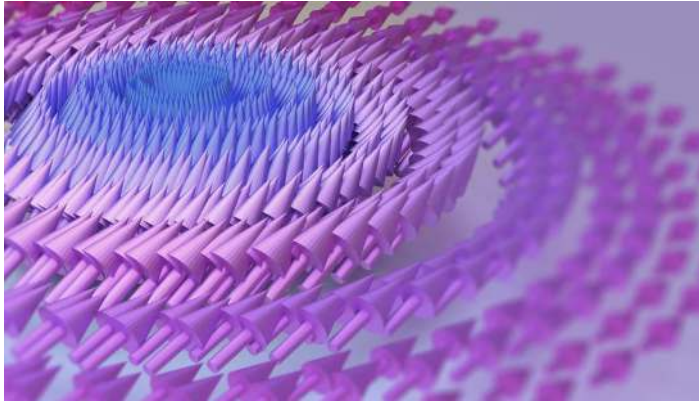


Catalysts

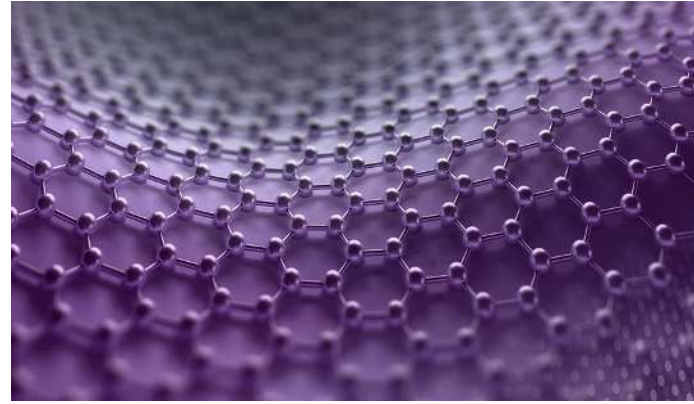


Metals, Ceramics & Glasses

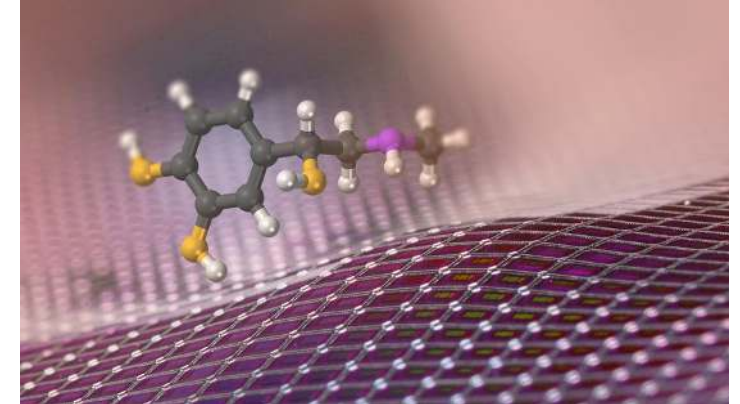
QuantumATK Addresses Key Materials Modeling Areas in Leading-Edge Semiconductor Development



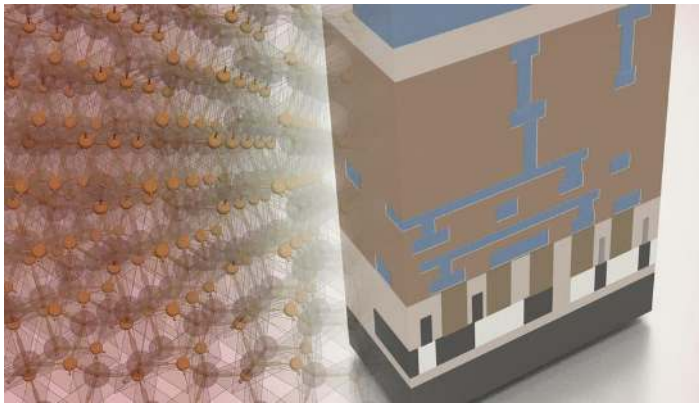
Spintronics & Novel Memory Devices



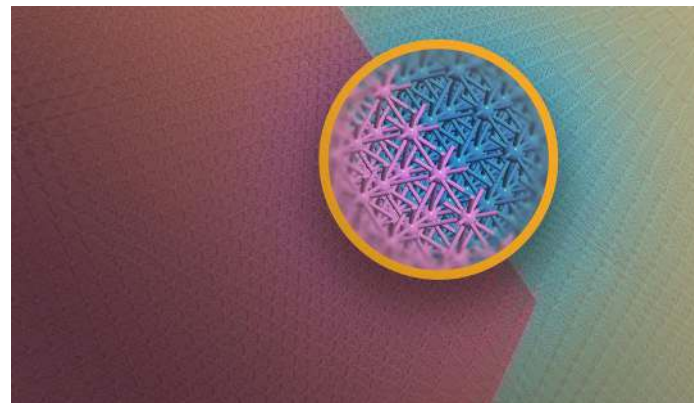
2D Material FET Performance



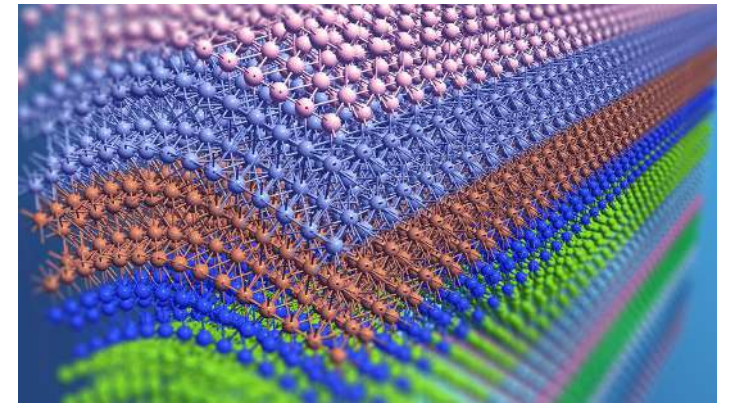
Surface Processes



Logic & Memory Interconnects



Metal-Semiconductor Contacts



High-K Metal Gates (HKMG) Stacks

Validated Platform And Methods

QuantumATK Reference Papers & Scientific Publications From User Base



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

Hemant Dixit, Chengyu Niu, Mark Raymond, Vimal Kamineni, Rajan K. Pandey, *Member, IEEE*, Anirudhha Konar, Jody Fronheiser, Adra V. Carr, Phil Oldiges, Praneet Adusumilli, Nicholas A. Lanzillo, Xin Miao, Bhagawan Sahu, and Francis Benistant

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Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci



ELSEVIER



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

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PHYSICAL REVIEW B 96, 195309 (2017)

First-principles Green's-function method for surface calculations: A pseudopotential localized basis set approach

Søren Smidstrup,^{1,2} Daniele Stradi,^{1,2} Jess Wellendorf,¹ Petr A. Khomyakov,¹ Ulrik G. Vej-Hansen,¹ Maeng-Eun Lee,¹ Tushar Ghosh,³ Elvar Jónsson,^{2,3} Hannes Jónsson,^{2,3} and Kurt Stokbro¹

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We present an efficient implementation of the Green's-function method for surface calculations within the framework of the pseudopotential localized basis set approach. In this method, the system is described by a reservoir, thereby overcoming the inherent difficulty of addressing the alignment in thin-film semiconductor surfaces in external electrical fields. The accuracy of the method is demonstrated by comparing experimental measurements and first-principles calculations.

DOI: 10.1103/PhysRevB.96.195309

I. INTRODUCTION

Atomic-scale modeling has established itself as a powerful tool in computational materials science. First-principles methods are routinely applied to study the chemical and physical properties of materials and their surfaces, including surface structures [1–6]. The surface calculations, which model a surface as a few atomic layers, has become the standard for first-principles atomic simulations despite the fact that a physical surface is not a simple slab of atoms, unless the surface ultrathin film or membrane is considered. A slab is by construction finite in the direction perpendicular to the surface plane, and therefore has a surface energy that is not always equivalent. As a consequence, the structure of the slab is not always representative of the bulk. This leads to a number of fundamental problems in the slab approach to model surfaces, the accuracy of which may critically depend on the slab thickness. This leads to a number of fundamental problems in the slab approach to model surfaces, the accuracy of which may critically depend on the slab thickness. This leads to a number of fundamental problems in the slab approach to model surfaces, the accuracy of which may critically depend on the slab thickness.

Abstract
ATK-ForceField is a new generation molecular dynamics software package. It is designed to be used in conjunction with QuantumATK, which is an integrated platform of electronic and atomic-scale modelling tools. The package will focus on geometry optimization, advanced modeling algorithms and three illustrative examples: a diatomic crystal, a vapor and a simulation of a diatomic crystal.

*stradi@synopsys.com

2469-9950/2017/96(19)195309(17)

OPEN ACCESS
IOP Publishing
Modelling and Simulation in Materials Science and Engineering
Modelling Simul. Mater. Sci. Eng. 25 (2017) 085007 (28pp)
<https://doi.org/10.1088/1361-651X/aa8810>

ATK-ForceField: a new generation molecular dynamics software package

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Journal of Physics: Condensed Matter
J. Phys.: Condens. Matter 32 (2020) 015901 (16pp)
<https://doi.org/10.1088/1361-648X/ab4007>

QuantumATK: an integrated platform of electronic and atomic-scale modelling tools

Søren Smidstrup¹, Troels Markussen¹, Pieter Vancraeyveld¹, Jess Wellendorf¹, Julian Schneider¹, Tue Gunst^{1,2}, Brecht Verstichel¹, Daniele Stradi¹, Petr A Khomyakov¹, Ulrik G Vej-Hansen¹, Maeng-Eun Lee¹, Samuel T Chill¹, Filip Rasmussen¹, Gabriele Penazzi¹, Fabiano Corsetti¹, Ari Ojanpera¹, Kristian Jensen¹, Mattias L N Palsgaard^{1,2}, Umberto Martinez¹, Anders Blom¹, Mads Brandbyge¹ and Kurt Stokbro¹

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Published 10 October 2019

Abstract
QuantumATK is an integrated set of atomic-scale modelling tools for professional software engineers in collaboration with academic researchers. While different professional software engineers in collaboration with academic researchers. While different professional software engineers in collaboration with academic researchers. While different professional software engineers in collaboration with academic researchers.

Published 10 October 2019
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[Phys. Rev. B 96 195309 \(2017\)](https://doi.org/10.1103/PhysRevB.96.195309)

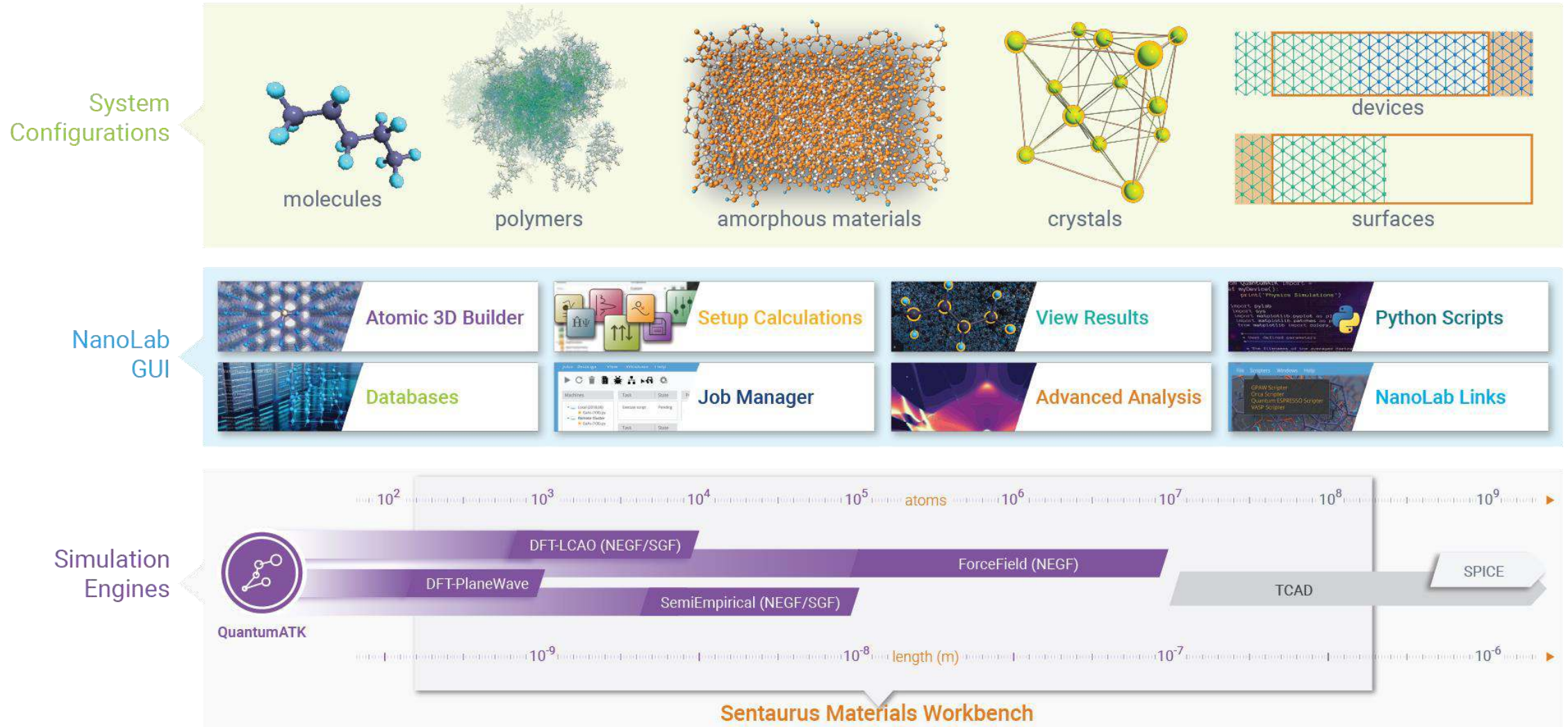
[Modelling Simul. Mater. Sci. Eng. 25 085007 \(2017\)](https://doi.org/10.1088/1361-651X/aa8810)

[J. Phys.: Condens. Matter 32 015901 \(2020\)](https://doi.org/10.1088/1361-648X/ab4007)

QuantumATK Atomic-Scale Modeling Platform



QuantumATK Atomic-Scale Modeling Platform



<https://www.synopsys.com/quantumatk>

QuantumATK Key Unique Features

GUI support for complicated simulation workflows

- Surface band structures, surface processes, composite MD flows, optical properties, ...

Interactive analysis of results and plotting

- Professional and intuitive GUI

Non-Equilibrium Green's-Function methods (NEGF)

- Unique functionalities to study realistic **surfaces** and **interfaces** (electrons reservoir, finite bias, no finite size effects, ...)
- Can be used with DFT or Semi-Empirical Methods

DFT with Linear Combination of Atomic Orbitals (LCAO)

- 2000+ atoms with modest hardware
- Also, at hybrid functional level (HSE, PBE0, B3LYP, ...)

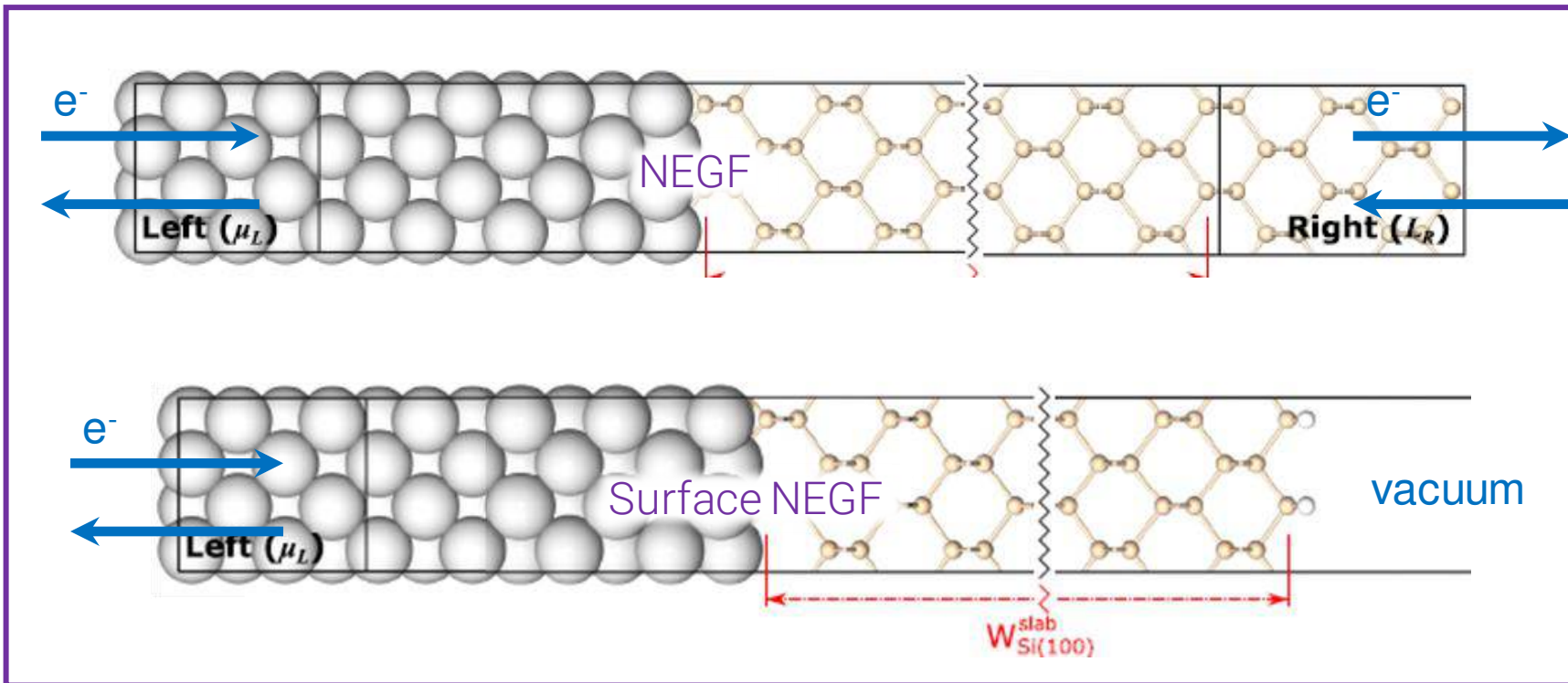
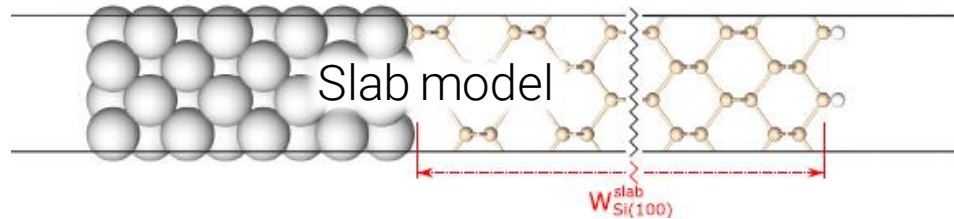
Machine-learned interatomic potentials

- Used for molecular-dynamics studies of materials for which no conventional potentials exist
- Nearly ab-initio accuracy, but orders of magnitude faster

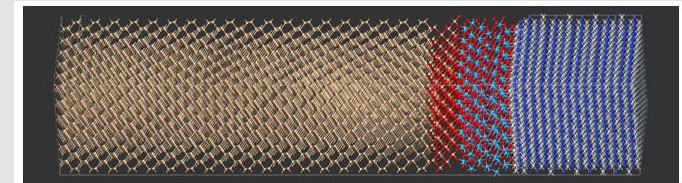
Seamless integration between all methods

- Easily mix DFT, SE, and FF simulations in one single flow, including on-the-fly analysis.
- Integration with TCAD

Non-Equilibrium Green's Function Methods For Simulating Realistic Interfaces And Surfaces



- ✓ Accurate tool to study interfaces & electronic devices
- ✓ No finite size and surface termination effects. No need for many layers (slab)
- ✓ Bias & gate to simulate resistance, capacitance and I-V characteristics
- ✓ Available with DFT and Semi-Empirical methods



Si|SiO₂|HfO₂|TiN
10,000 atoms with DFT

Highly Efficient Hybrid Functionals with LCAO

- HSE-LCAO enables fast **2000+ atoms simulations**
 - Performance comparable to ordinary GGA/LDA
 - Possible without supercomputers
 - Beyond 3500 atoms on 64 cores in less than a day
 - **Screen new materials and processes wider and faster**

Unique methods enable **fast** computation



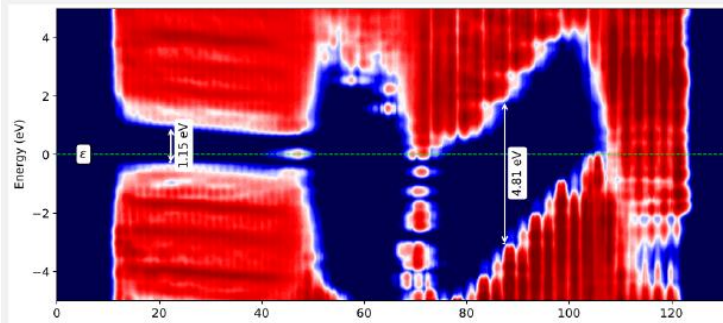
Amorphous Poly(ethyleneoxide)

Method	Time for full SCF to convergence*
LCAO-PBE	38m
LCAO-HSE06	1h2m16s

3560 atoms
16 MPI processes, 2 OMP threads

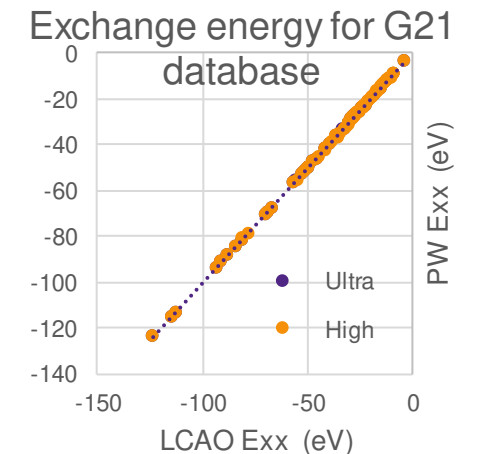
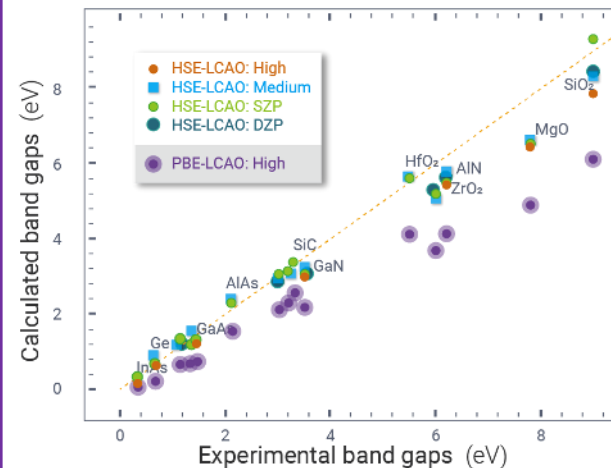
HSE-LCAO for **complex interfaces**

Si-SiO₂-HfO₂-TiN (1969 atoms), HSE06, SZP



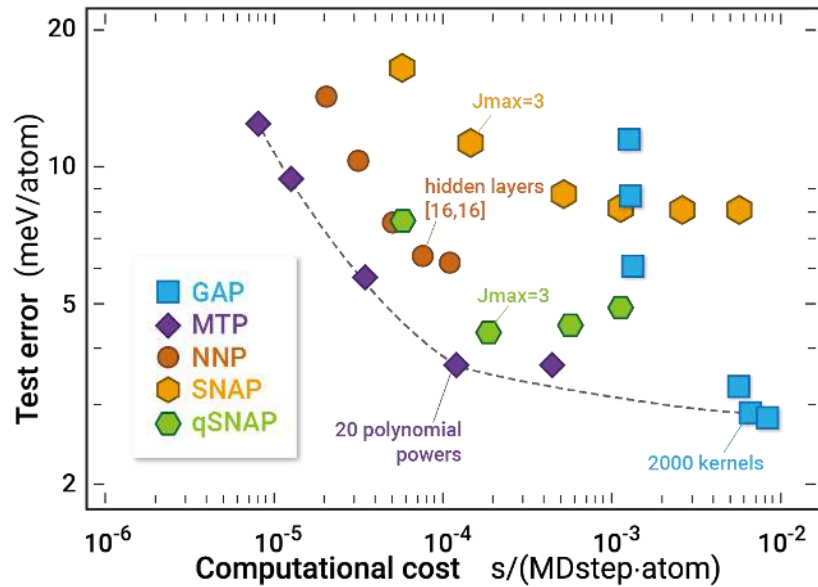
- Band gaps
- Defect levels
- Band bending
- Multiple interfaces
- Interface states
- 16h on 24 cores

HSE-LCAO gives similar **accuracy** as HSE-PW

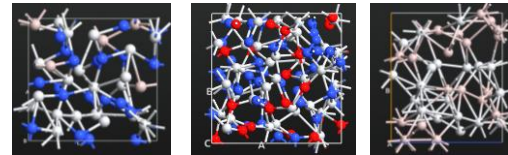


Moment Tensor Potentials (MTP)

Machine-Learned Interatomic Potentials for High QOR at Low TAT

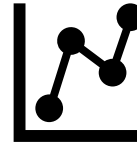


Full MTP flow integrated in one single software platform



Training configurations

Ab-initio PES



ML training



MTP ready to be used

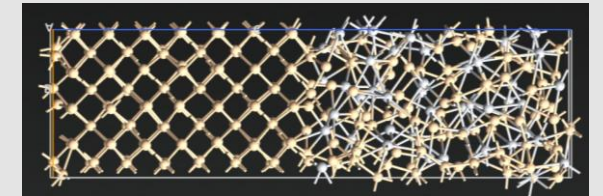
✓ Used for materials for which no conventional potentials exist

✓ Nearly *ab-initio* accuracy, but orders of magnitude faster

✓ Systematically improveable

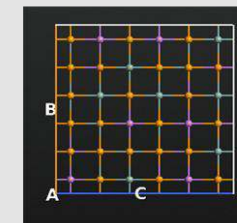
Crystalline Si

Amorphous TiSi

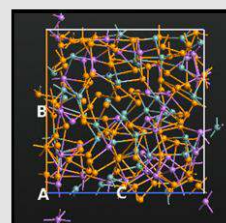


Crystalline GST

Amorphous GST



DFT-MD (2d9h)
FBMC (1d5h)
MTP (1h)



MTP [1,2] is one of the most accurate and efficient ML potentials on the market

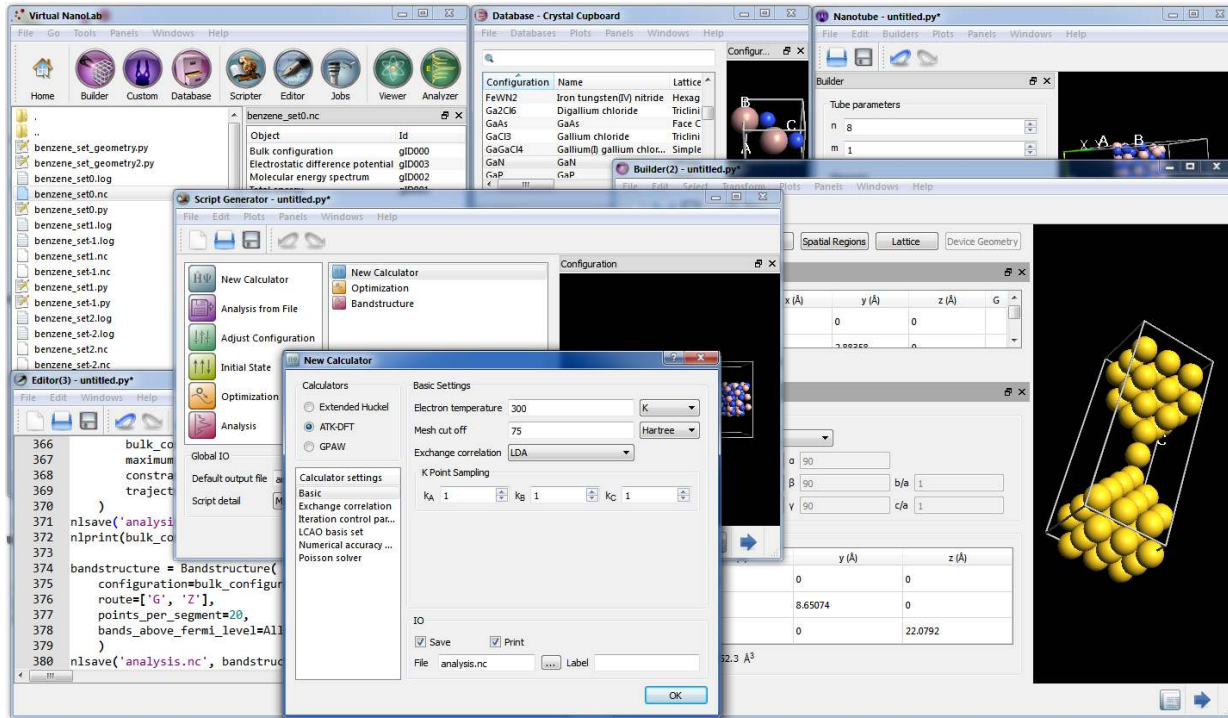
[1] A. V. Shapeev, Mult. Model. Sim. (2016)

[2] Y. Zuo et al., J. Phys. Chem. A 124, 731 (2020)

Easy Of Use Vs. Expert Users

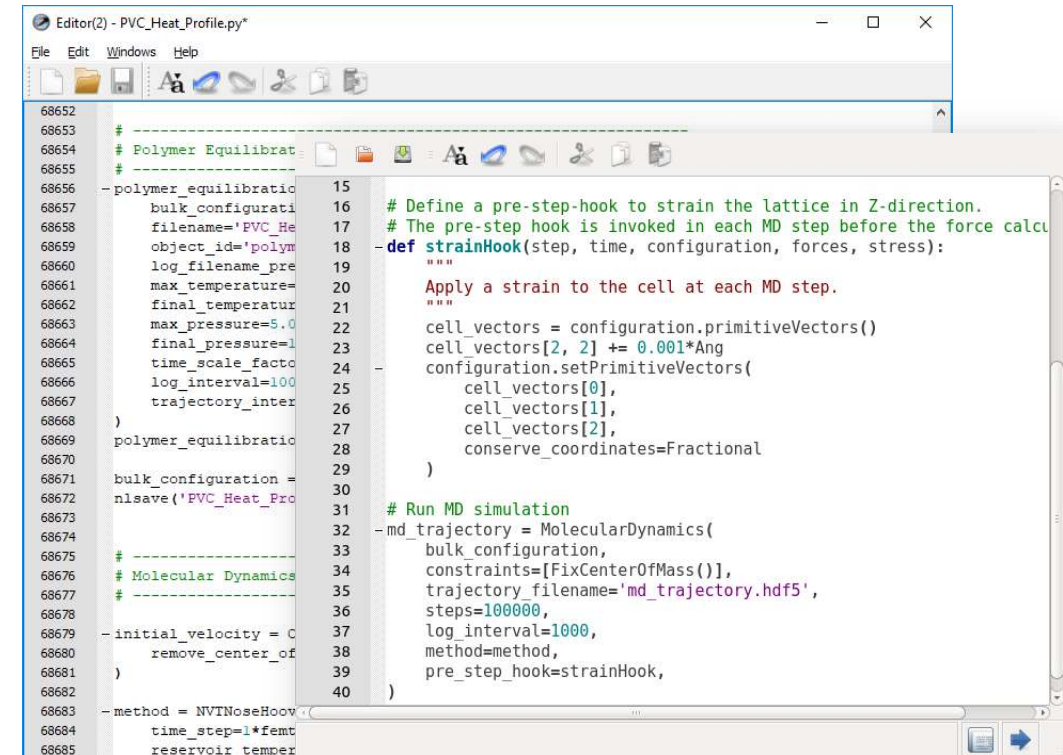
Graphical mode

- Intuitive interface
- Ready-to-use material databases
- Predefined workflows & templates



Scripting Mode

- GUI-based Python scripting
- Automate tasks
- Customize workflows & templates



Learn More about QuantumATK

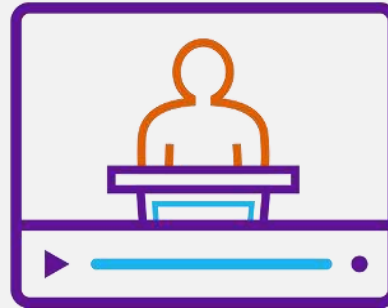


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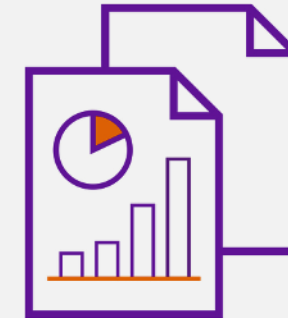
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