SYNOPSYS®
Silicon to Software™

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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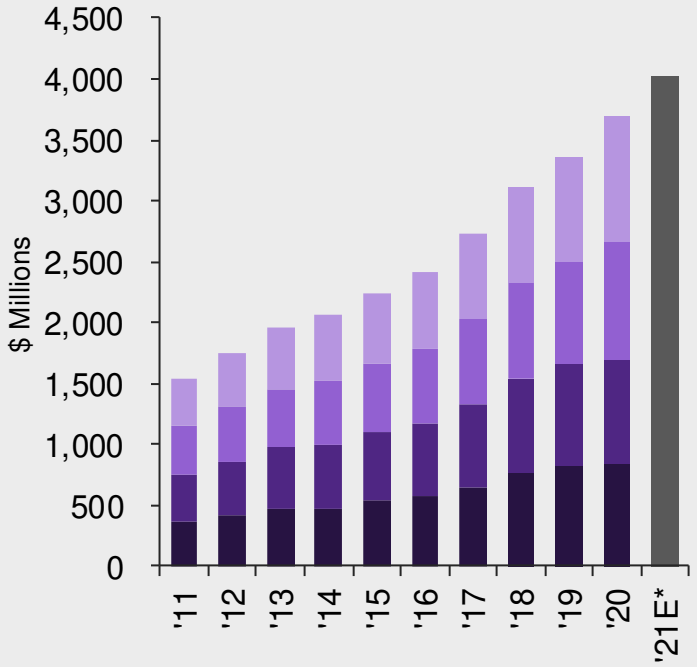
Synopsys Today: From Silicon to Software

FY20 Revenue: ~$3.7B

Employees: ~15,000

Patents: ~3,300

Offices: ~125

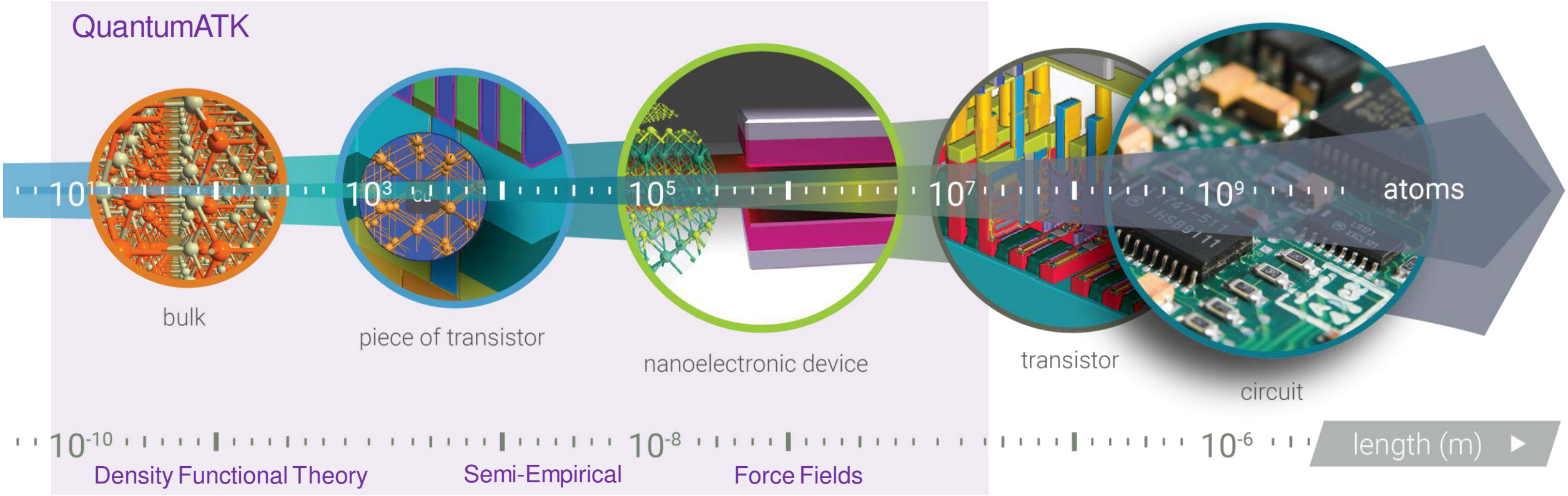


#1 electronic design automation tools & services

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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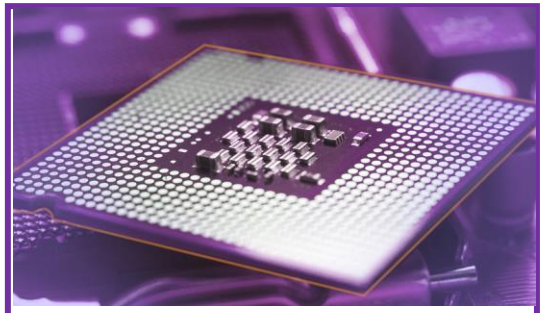
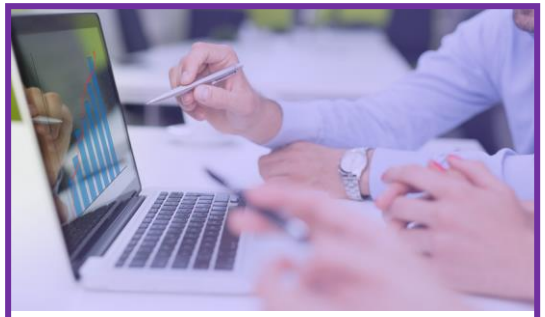
Atomic-Scale Modeling Benefits



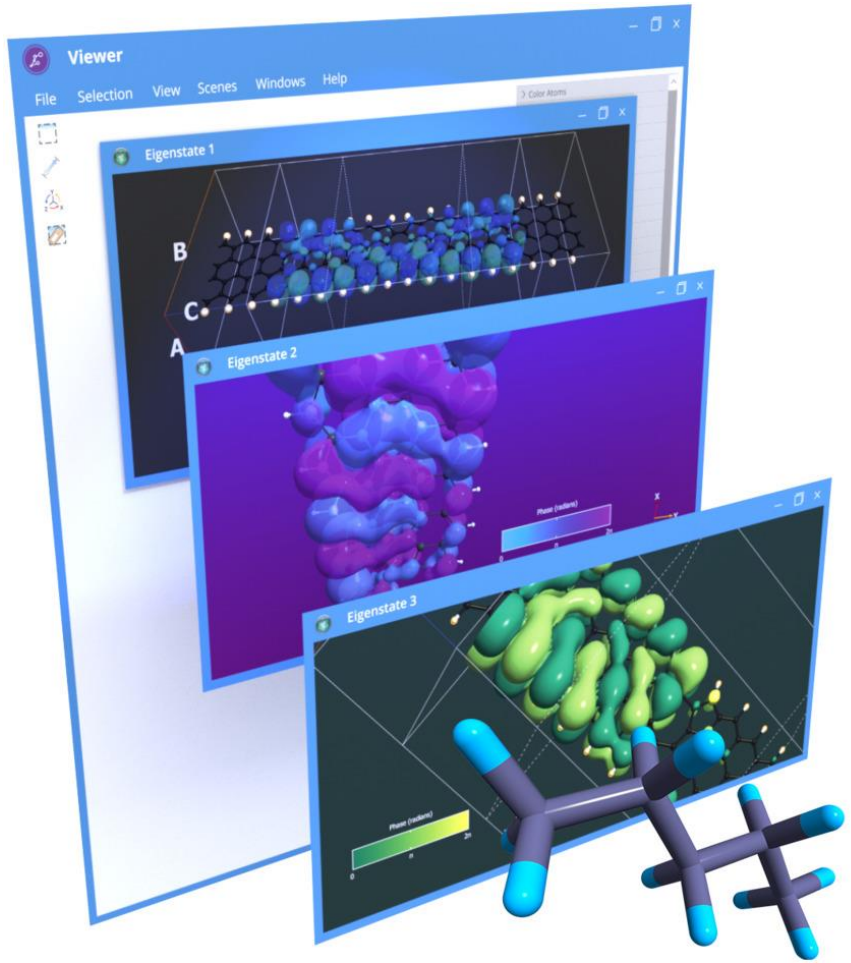
Helps in path finding for solving current industrial problems

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.

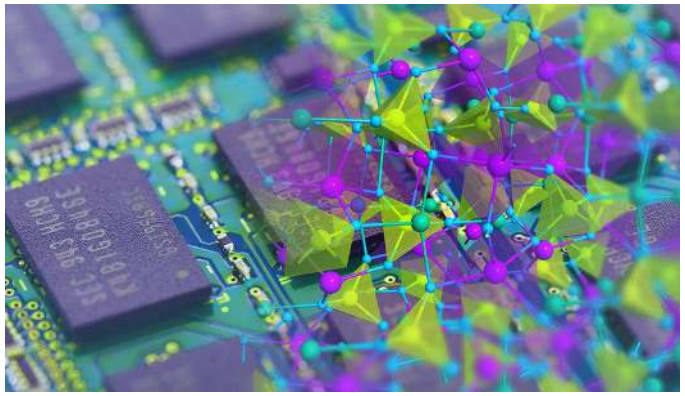
2. Synergistic Solution

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

3. Realistic Physics Outcomes in Complex Materials

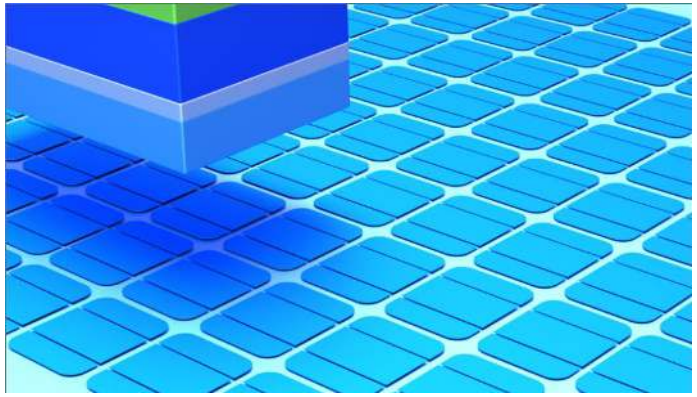
- ✓ Strong capability to analyze **large scale systems** and thus provide more realistic simulation results
- ✓ Unique features for electron **transport**

QuantumATK Addresses Key Materials Modeling Areas



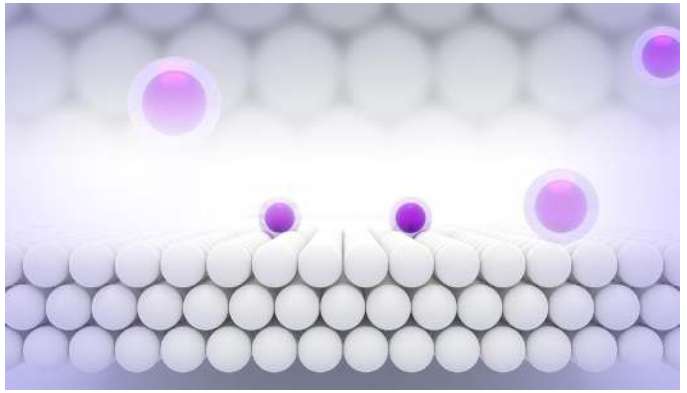
Semiconductors

Batteries

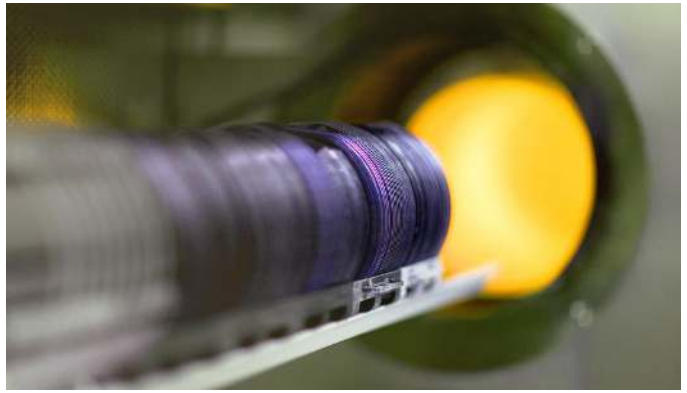


Solar & Fuel Cells

Polymers

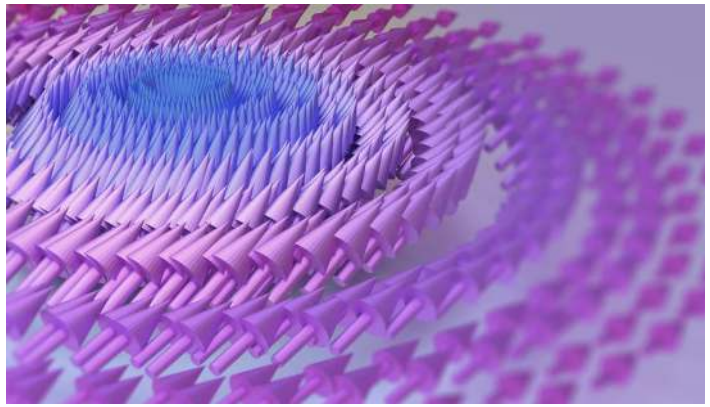


Catalysts

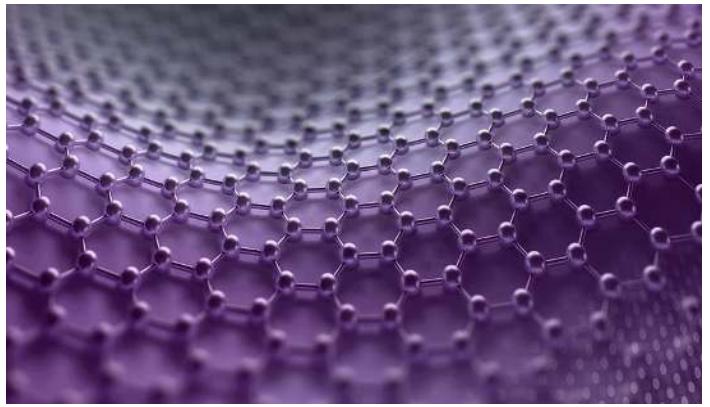


Metals, Ceramics & Glasses

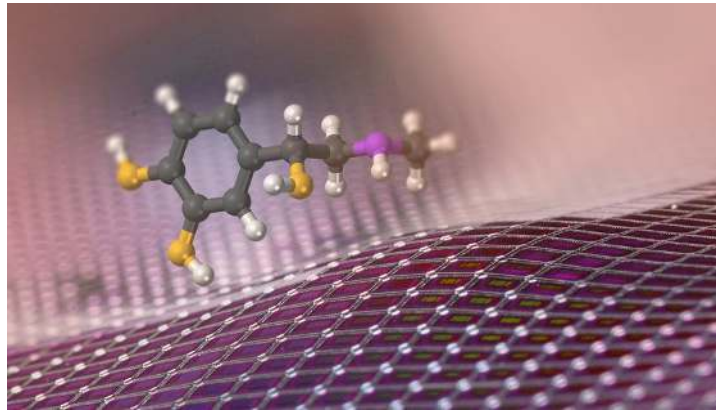
QuantumATK Addresses Key Materials Modeling Areas in Leading-Edge Semiconductor Development



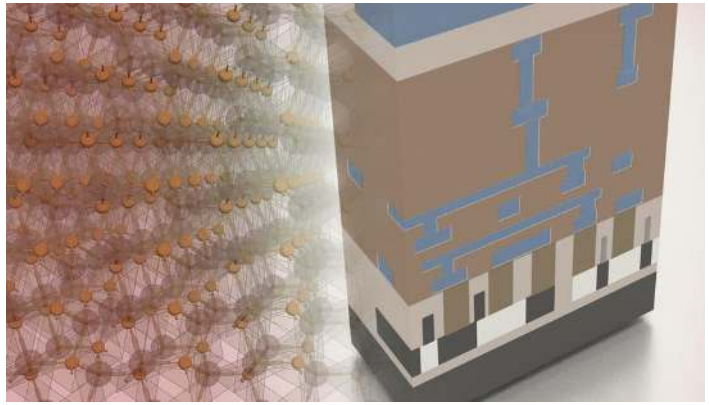
Spintronics & Novel Memory Devices



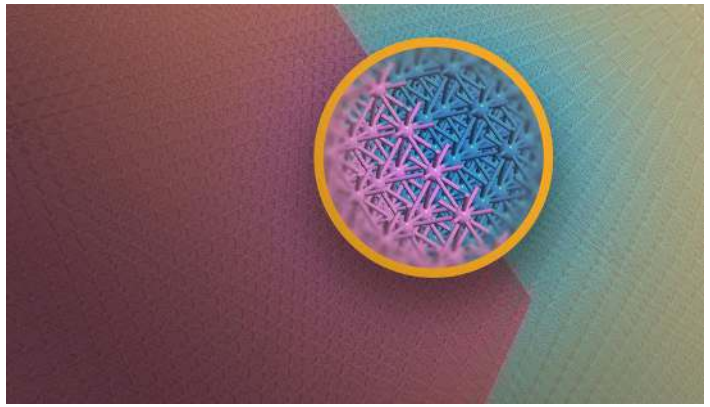
2D Material FET Performance



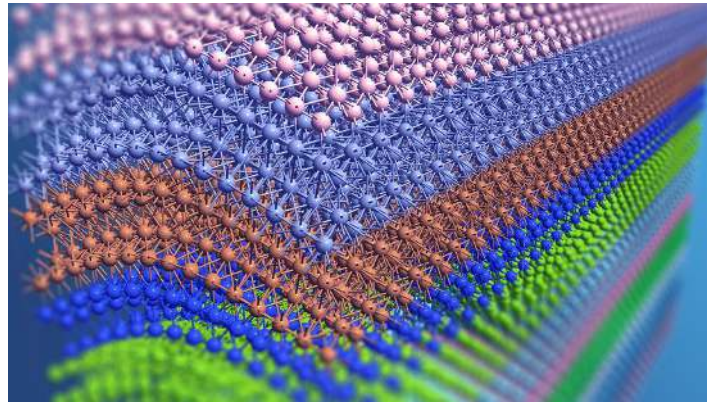
Surface Processes



Logic & Memory Interconnects



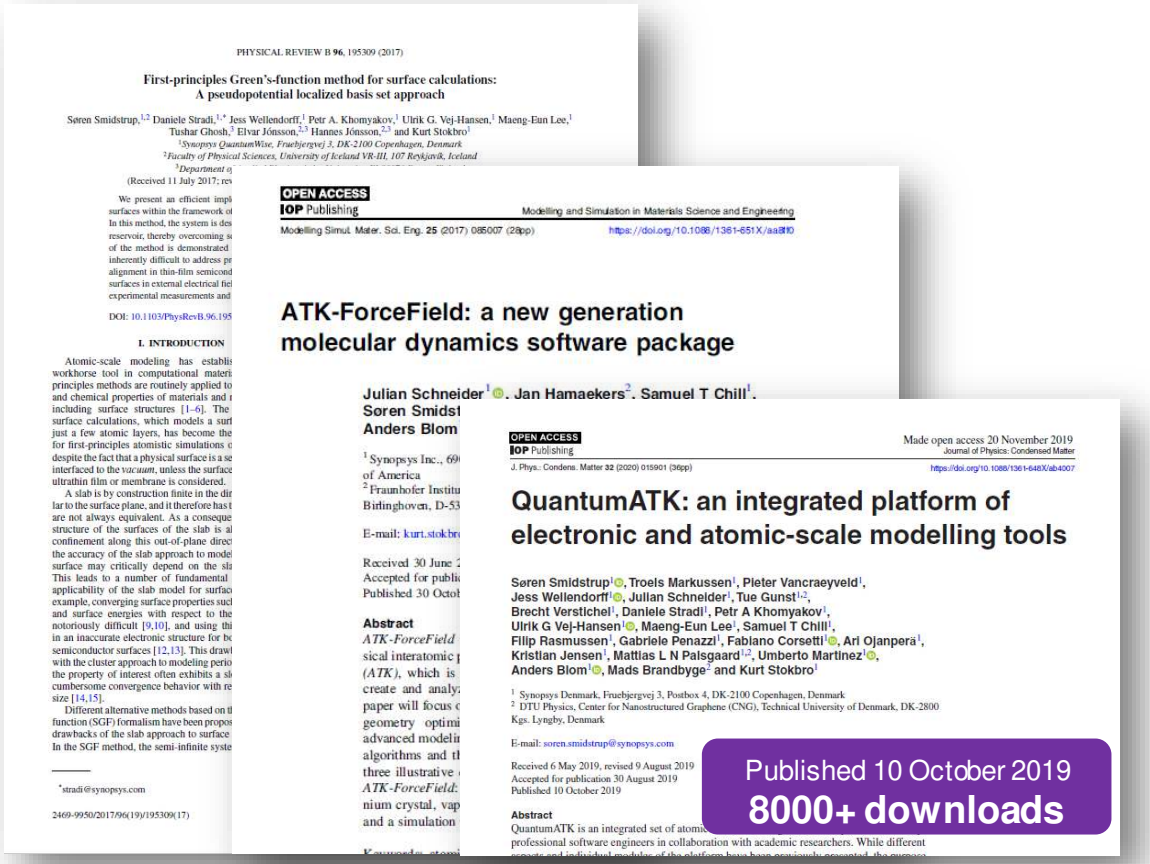
Metal-Semiconductor Contacts



High-K Metal Gates (HKMG) Stacks

Validated Platform And Methods

QuantumATK Reference Papers & Scientific Publications From User Base



PHYSICAL REVIEW B 96, 195309 (2017)

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

OPEN ACCESS
IOP Publishing
Modelling and Simulation in Materials Science and Engineering
Modelling Simul. Mater. Sci. Eng. 25 (2017) 085007 (28pp)

ATK-ForceField: a new generation molecular dynamics software package

OPEN ACCESS
IOP Publishing
Made open access 20 November 2019
Journal of Physics: Condensed Matter
J. Phys.: Condens. Matter 32 (2020) 015901 (36pp)

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

Published 10 October 2019
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[Phys. Rev. B **96** 195309 (2017)]
[Modelling Simul. Mater. Sci. Eng. **25** 085007 (2017)]
[J. Phys.: Condens. Matter **32** 015901 (2020)]

IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 64, NO. 9, SEPTEMBER 2017 3775

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

2400+ publications using QuantumATK

Contents lists available at ScienceDirect

Computational Materials Science

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

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

Nicholas A. Lanzillo[a,*], Benjamin D. Briggs[a], Robert R. Robison[a], Theo Standaert[a], Christian Lavoie[b]

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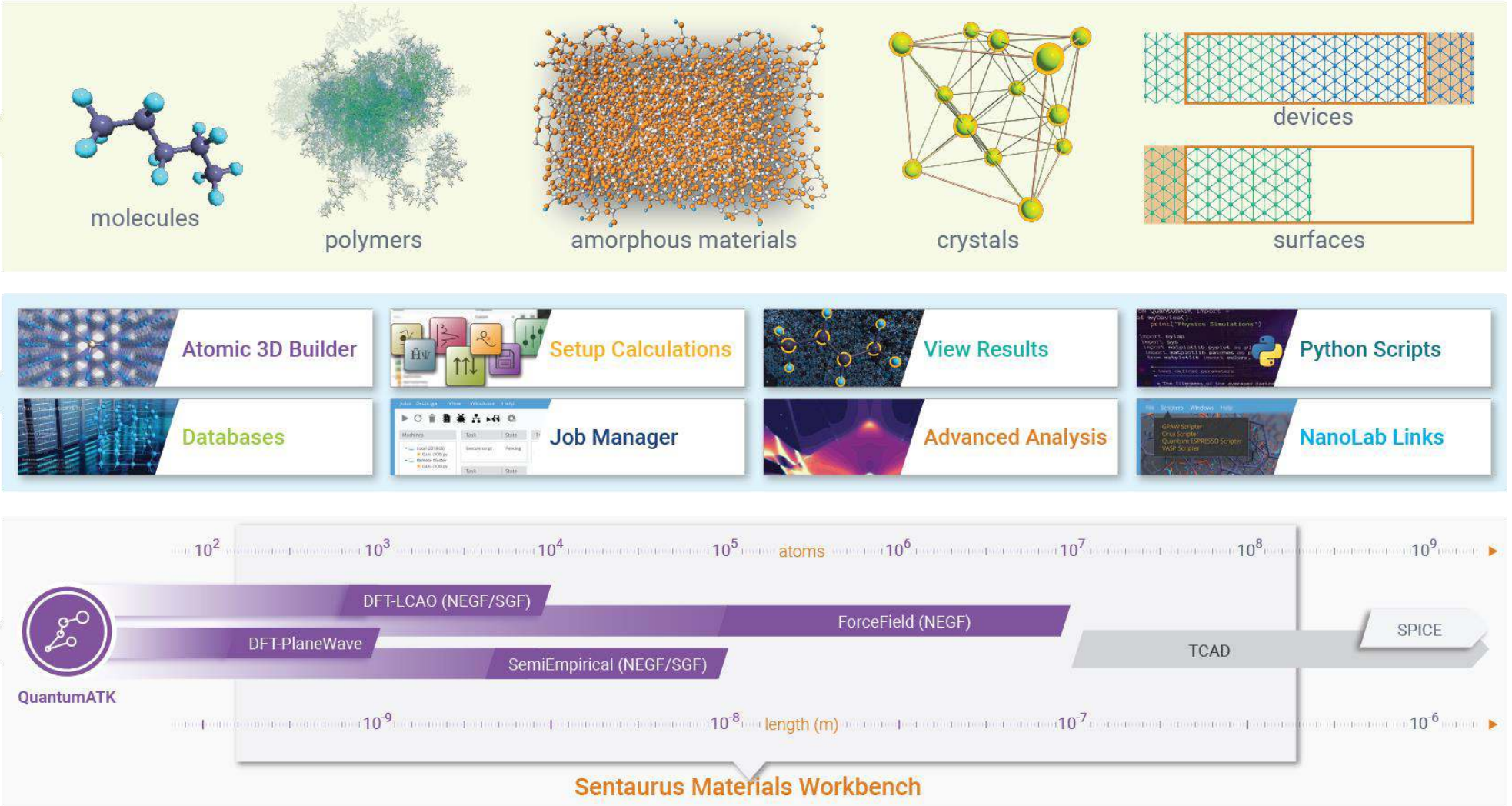
QuantumATK Atomic-Scale Modeling Platform

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

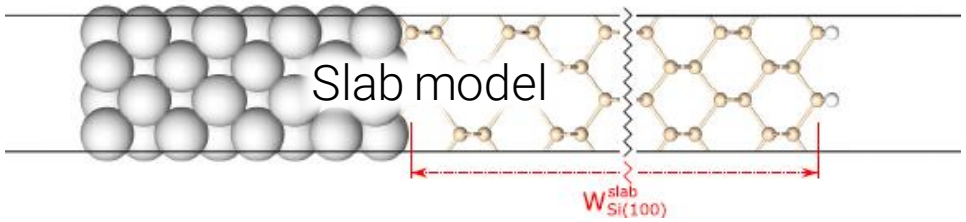
DFT with Linear Combination of Atomic Orbitals (LCAO)
- 2000+ atoms with modest hardware
- Also, at hybrid functional level (HSE, PBE0, B3LYP, …)

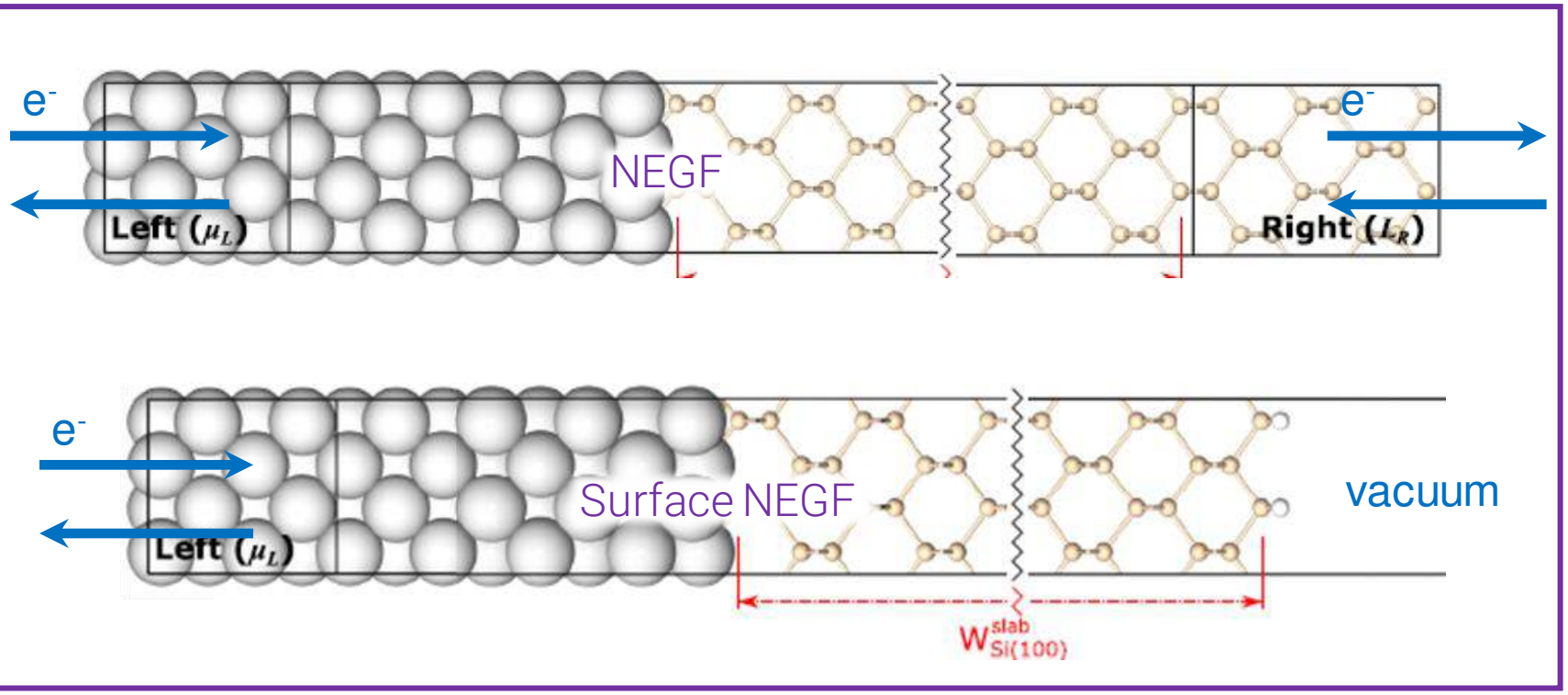
Machine-learned interatomic potentials
- Used for molecular-dynamics studies of materials for which no conventional potentials exist
- Nearly ab-initio accuracy, but orders of magnitude faster

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

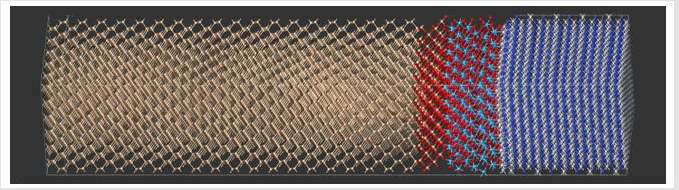
Non-Equilibrium Green's Function Methods

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



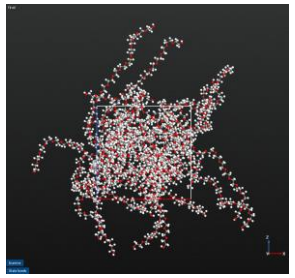
$Si|SiO_2|HfO_2|TiN$

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



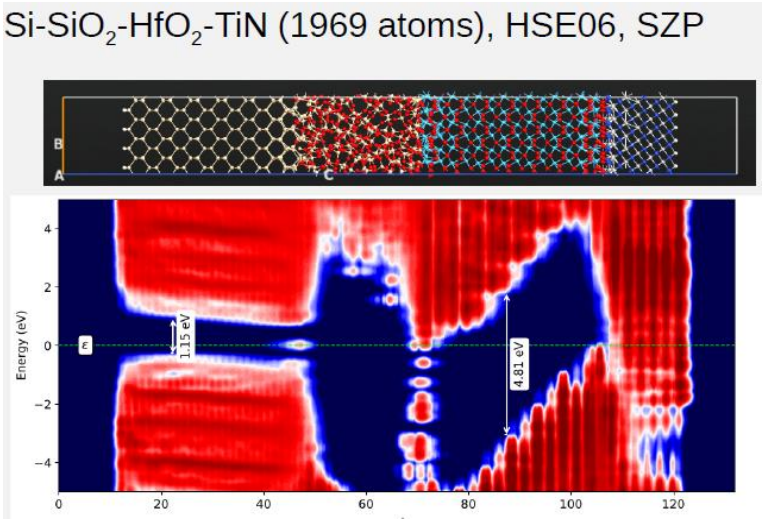
Amorphous
Poly(ethyleneoxide)

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

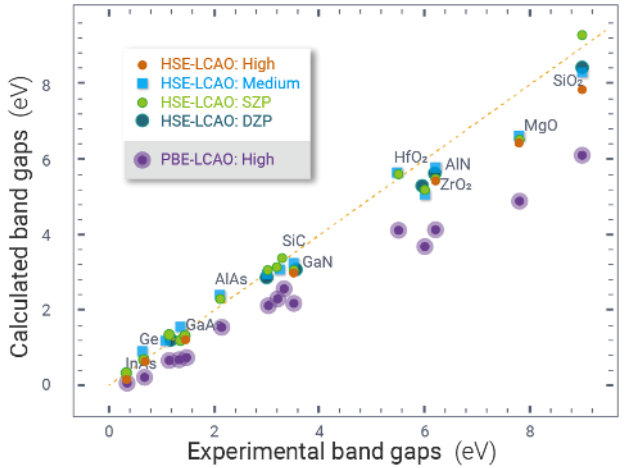
3560 atoms
16 MPI processes, 2 OMP threads

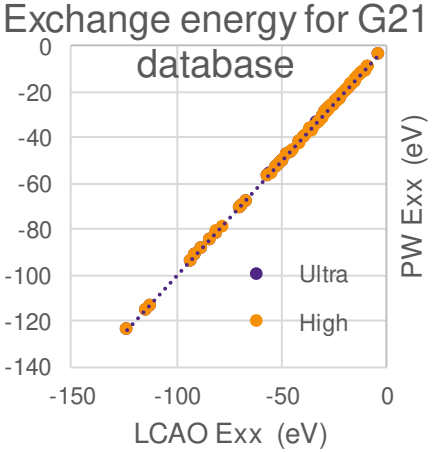
HSE-LCAO for **complex interfaces**

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



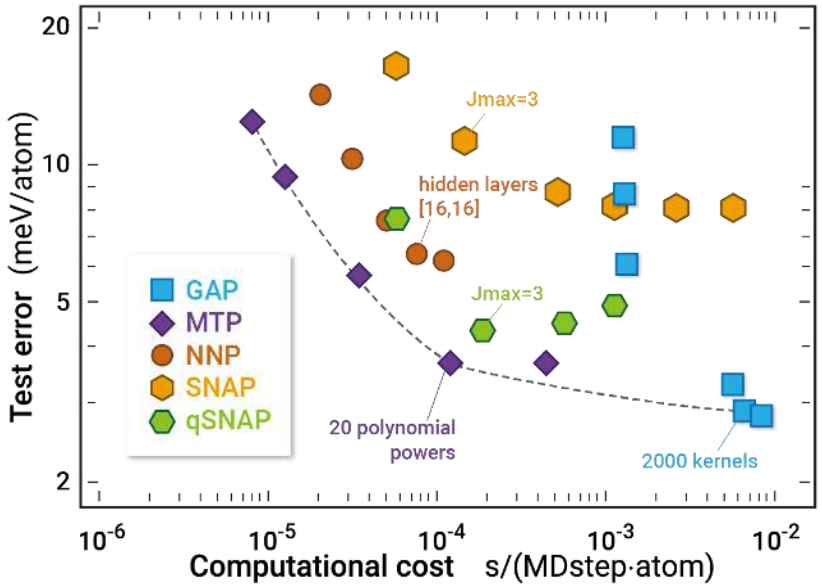
HSE-LCAO gives similar **accuracy** as HSE-PW





Moment Tensor Potentials (MTP)

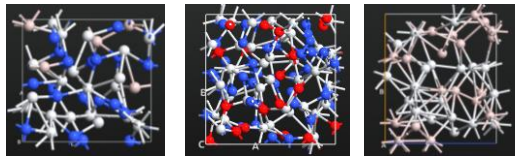
Machine-Learned Interatomic Potentials for High QOR at Low TAT



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)

Full MTP flow integrated in one single software platform



Training configurations

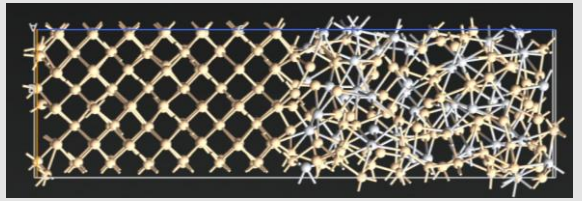
Ab-initio PES

ML training

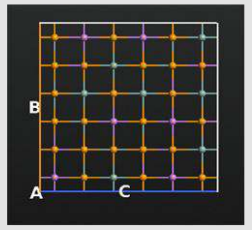
MTP ready to be used

- ✓ Used for materials for which no conventional potentials exist
- ✓ Nearly *ab-initio* accuracy, but orders of magnitude faster
- ✓ Systemtically improveable

Crystalline Si Amorphous TiSi

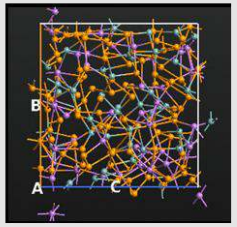


Crystalline GST



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

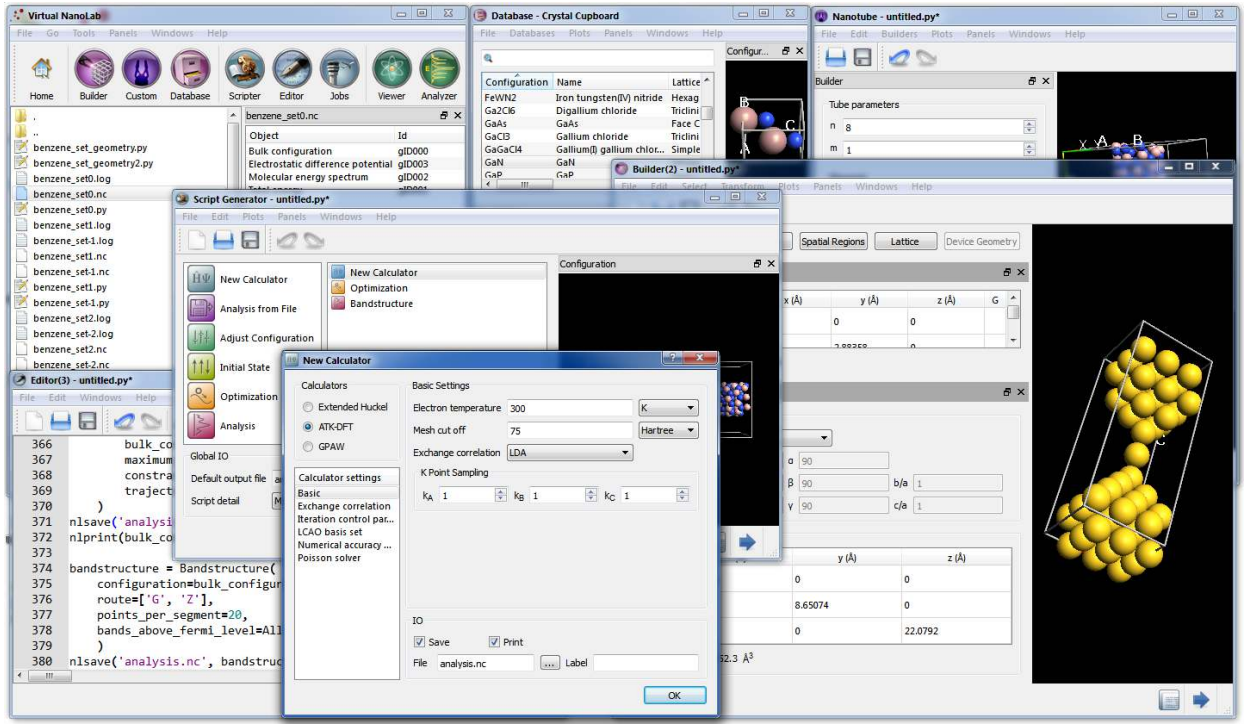
Amorphous GST



Easy Of Use Vs. Expert Users

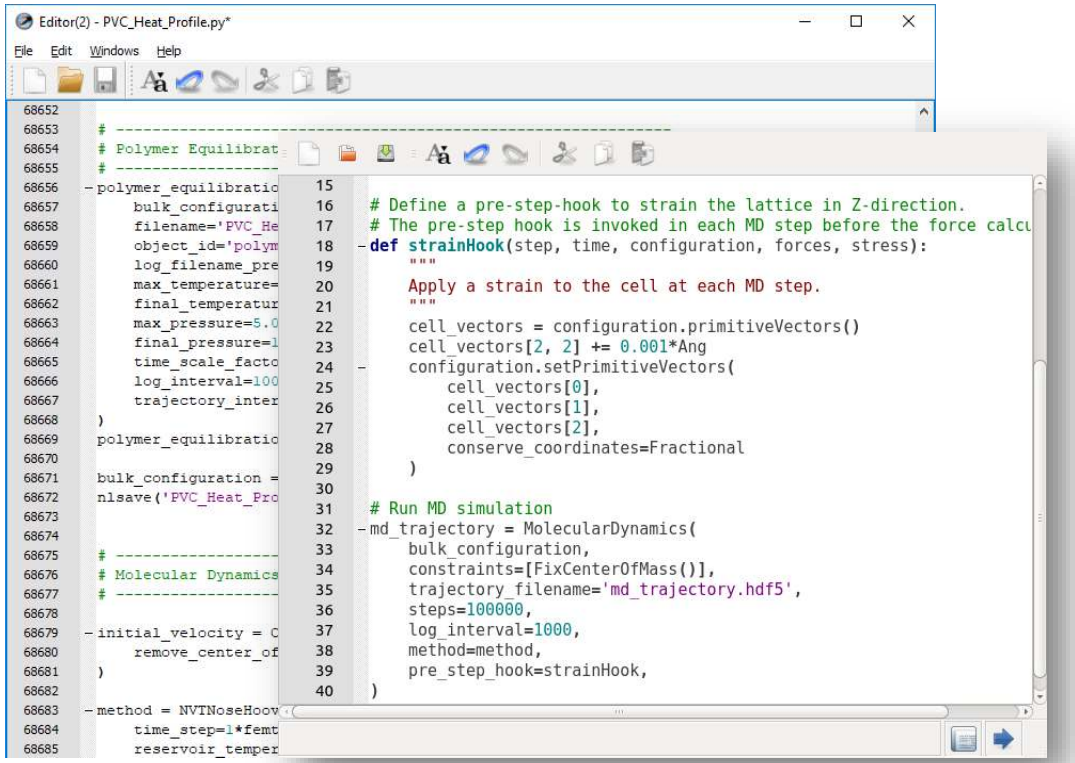
Graphical mode

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



Scripting Mode

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



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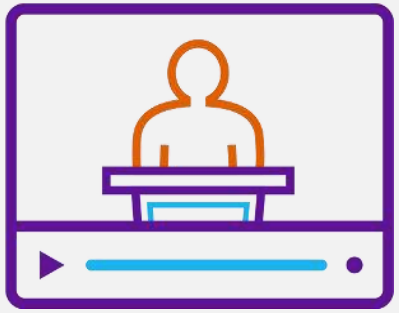
Academic Research Program in Europe: Europractice



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