Electronic structure theory on the world market

Kurt Stokbro, QuantumWise A/S

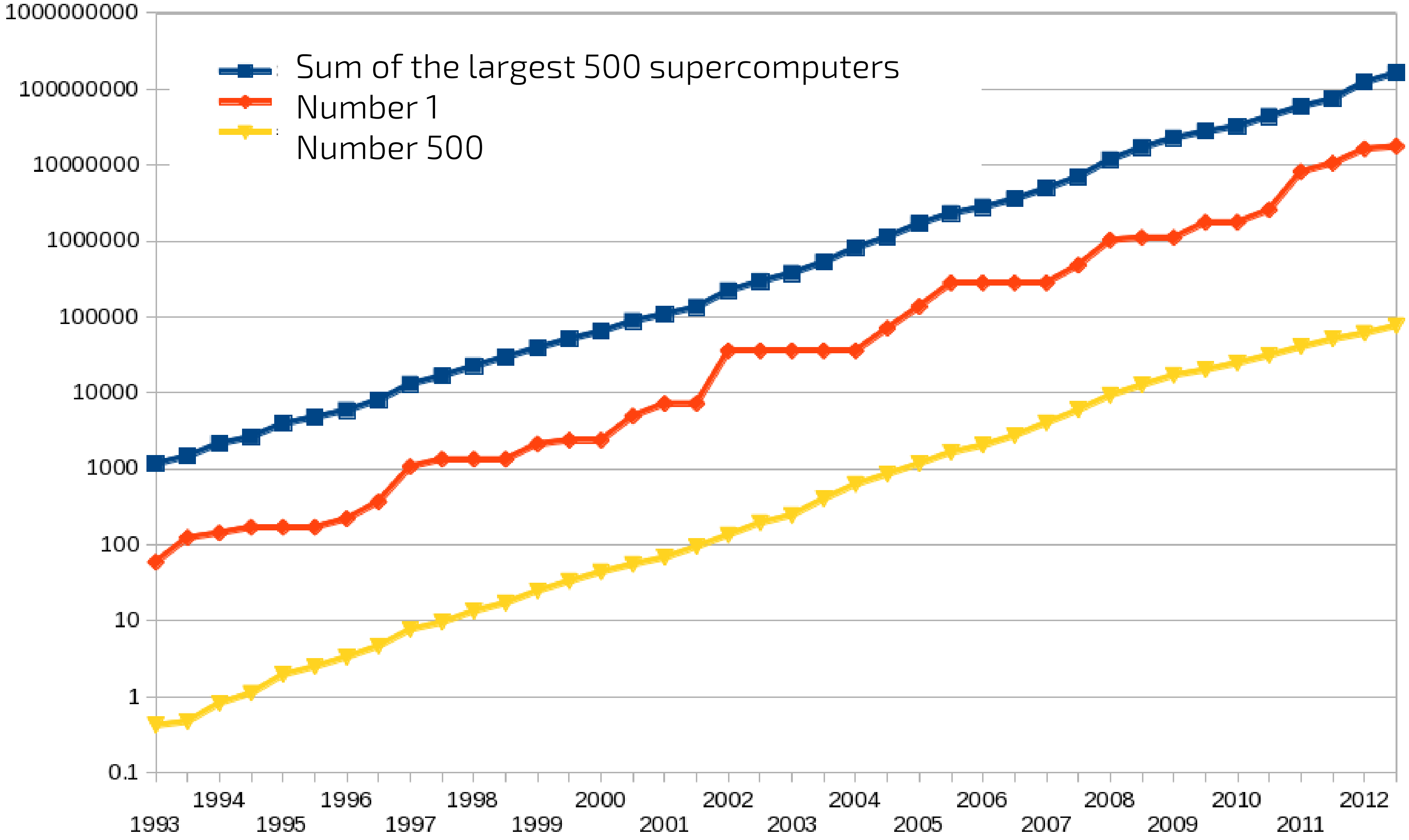
Kurt Stokbro

QuantumWise

Most cited papers in APS (from 1893)

	Journal	# cites	Title	Author(s)
1	PRB (1988)	39190	Development of the Colle-Salvetti Correlation-Energy …	Lee, Yang, Parr
2	PRL (1996)	25452	Generalized Gradient Approximation Made Simple	Perdew, Burke, Ernzerhof
3	PRA (1988)	22904	Density-Functional Exchange-Energy Approximation …	Becke
4	PR (1965)	20142	Self-Consistent Equations Including Exchange and Correlation …	Kohn and Sham
5	PRB (1996)	13731	Efficient Iterative Schemes for Ab Initio Total-Energy …	Kresse and Furthmuller
6	PRB (1976)	13160	Special Points for Brillouin-Zone Integrations	Monkhorst and Pack
7	PRB (1992)	10876	Accurate and Simple Analytic Representation of the Electron …	Perdew and Wang
8	PRB (1999)	10007	From Ultrasoft Pseudopotentials to the Projector Augmented …	Kresse and Joubert
9	PRB (1990)	9840	Soft Self-Consistent Pseudopotentials in a Generalized …	Vanderbilt
10	PR (1964)	9789	Inhomogeneous Electron Gas	Hohenberg and Kohn
11	PRB (1981)	9787	Self-Interaction Correction to Density-Functional Approx. …	Perdew and Zunger
12	PRB (1992)	9786	Atoms, Molecules, Solids, and Surfaces - Applications of the …	Perdew, Chevary, …
13	PRB (1986)	9313	Density-Functional Approx. for the Correlation-Energy …	Perdew
14	PR (1934)	9271	Note on an Approximation Treatment for Many-Electron Systems	Moller and Plesset
15	PRB (1994)	9100	Projector Augmented-Wave Method	Blochl
16	PRL (1980)	7751	Ground-State of the Electron-Gas by a Stochastic Method	Ceperley and Alder
17	PRL (1987)	7663	Inhibited Spontaneous Emission in Solid-State Physics …	Yablonovitch
18	PRL (1986)	7589	Atomic Force Microscope	Binnig, Quate, Gerber
19	PRB (1991)	7425	Efficient Pseudopotentials for Plane-Wave Calculations	Troullier and Martins
20	PRB (1993)	6925	Ab initio Molecular Dynamics for Liquid Metals	Kresse and Hafner
21	PR (1961)	6467	Effects of Configuration Interaction on Intensities and Phase Shifts	Fano
22	PR (1957)	6260	Theory of Superconductivity	Bardeen, Cooper, Schrieffer

Computing power 1993-2013



Computing power doubles every 14 months

Questions

Who are using electronic structure methods ?

Academia/Industry

What are they using the tools for ?

Application areas

How to answer these questions?

- Stastics summer school
- Statistics of publications
- *"The economic impact of molecular modelling of chemicals and materials"*, Goldbeck consulting
- QuantumWise user base

Participants at summer school

2014: 125 participants
29 nationalities

Denmark	**33**
China	11
Germany	10
Italy	8
United States	8
India	7
France	6
Iceland	4
Spain	4
United Kingdom	4
Finland	3

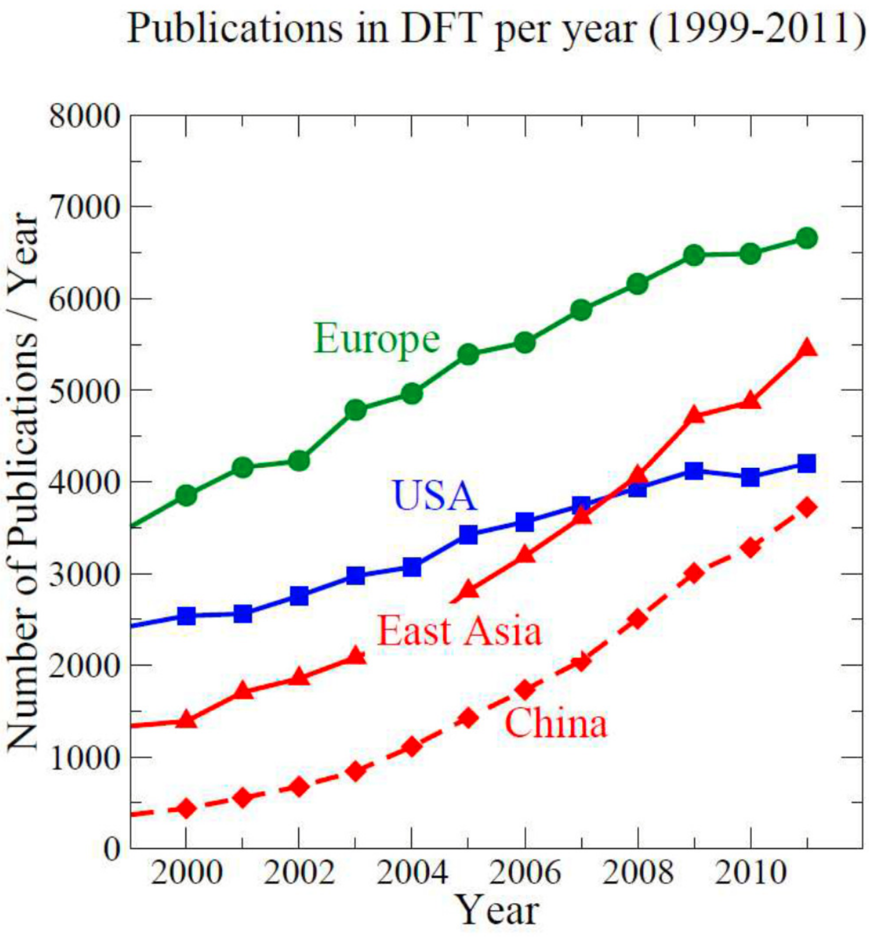
Europe 66%
Male 82 %

2016: 161 participants
35 nationalities

Denmark	**27**
Germany	21
United States	19
China	15
Italy	11
South Korea	9
India	9
United Kingdom	7
Sweden	5
Russia	3

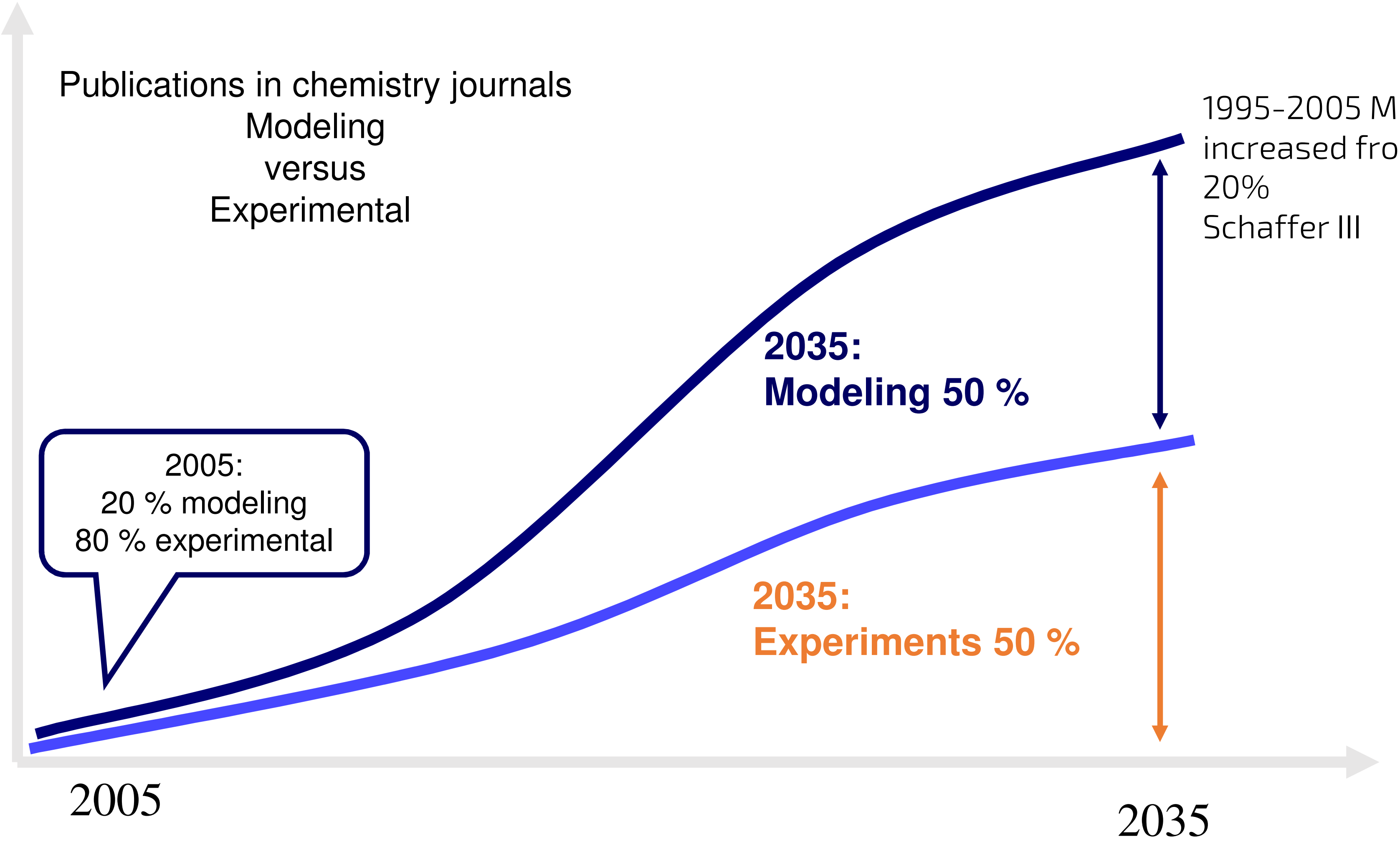
Europe 56%
Male 80 %

World activity in DFT in terms of publications



Source: Peter H Dederichs and Phivos Mavropoulos, Forschungszentrum Jülich.

The use of modeling software tools is increasing rapidly



Publications in chemistry journals
Modeling
versus
Experimental

2005:
20 % modeling
80 % experimental

2035:
Modeling 50 %

2035:
Experiments 50 %

2005

2035

1995-2005 Modeling increased from 10% to 20%
Schaffer III

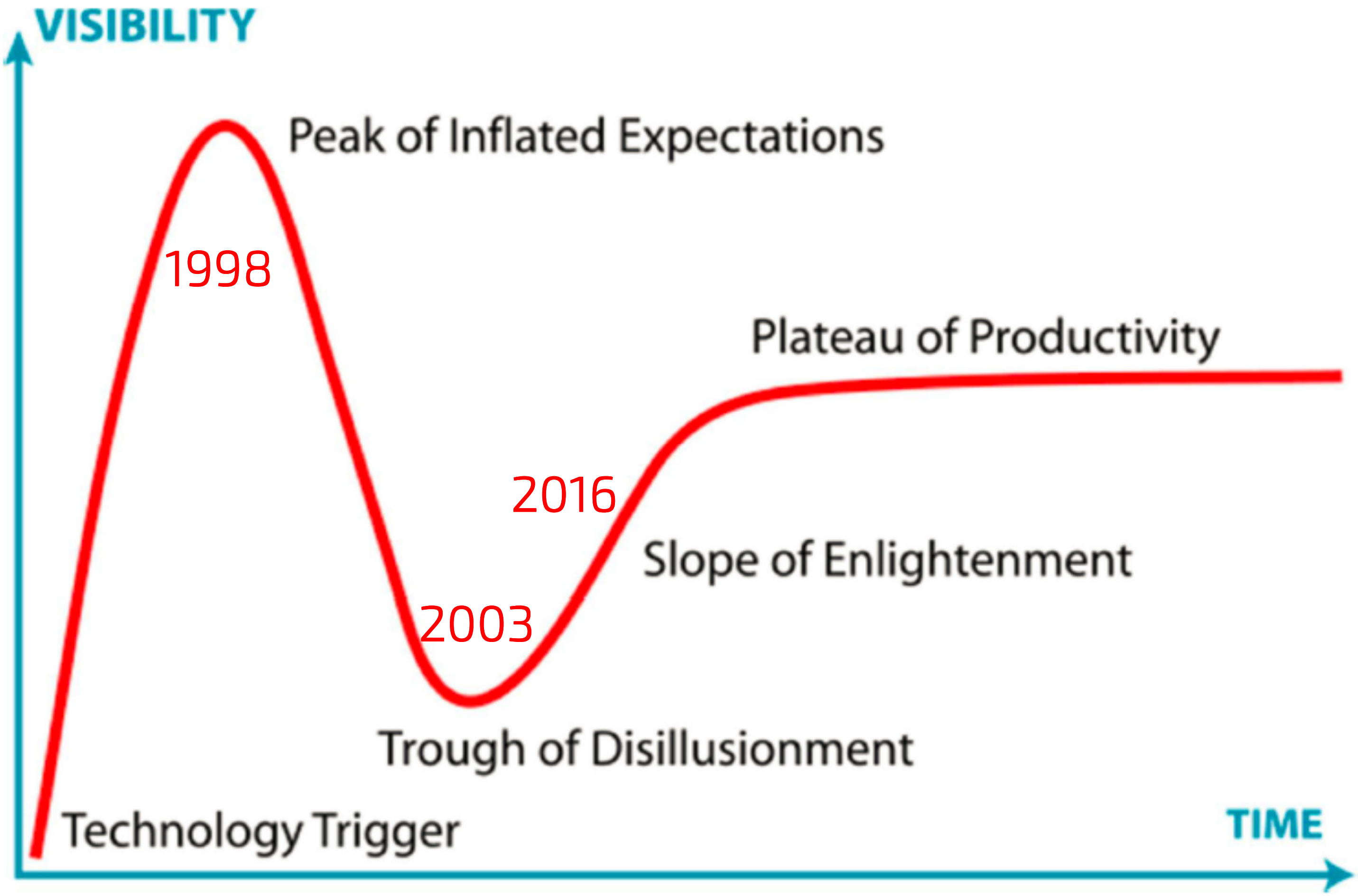
Industrial Users

- **Chemical** – major chemical companies have modeling groups since the 1980's using discrete models; modelling of solid state systems (heterogeneous catalysis) started later; smaller chemical companies are still in the process of adopting discrete models
- **Electronic** – leading electronics companies have been pioneering discrete models on the electronic and atomistic levels since the 1970's (IBM, NEC, Bell Labs); today major players like Intel, Samsung, Fujitsu, Panasonic, TSMC use commercial e/a software
- **Automotive** – leading companies like Toyota, Honda, GM have been using e/a modelling in-house since several decades; European car companies are in the process of adopting e/a modelling
- **Oil, gas, energy** – leading companies like Shell and ExxonMobil have in-house modelling groups using e/a models; government supported research organizations (IFPEN, Mexian Petroleum Institute) support industrial efforts
- **Other** –

KS1

Industrial impact

Measuring heat of formation for a single molecule is 50 times more expensive than accurate Quantum Chemistry calculations



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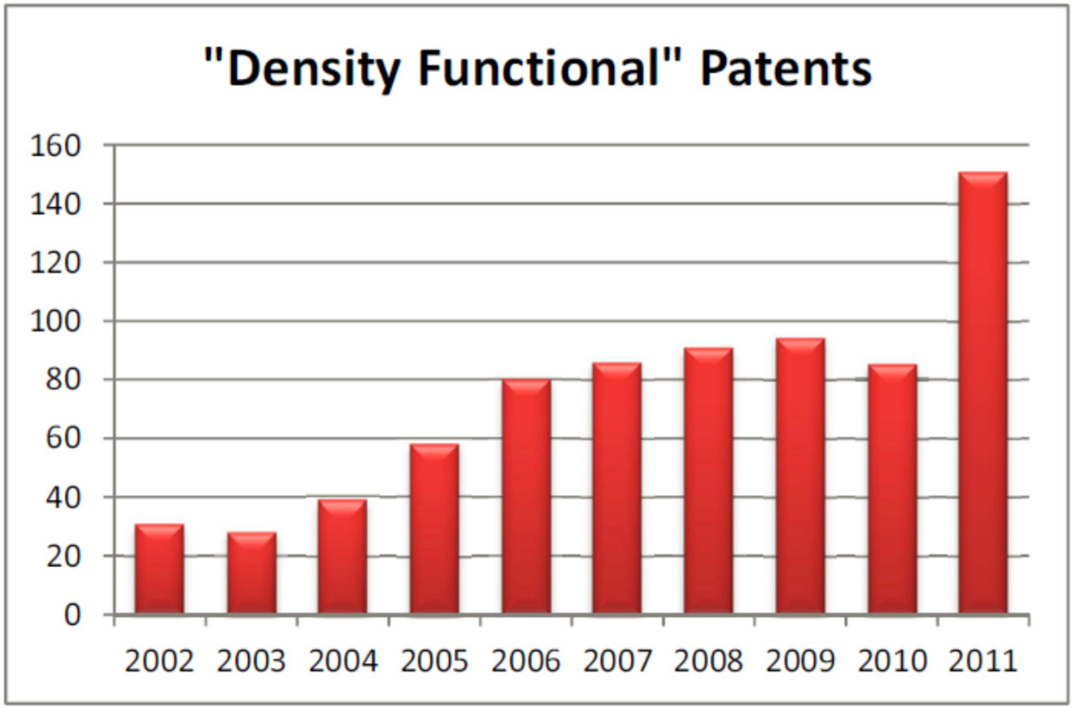
KS1 Kurt Stokbro; 14-08-2016

Patents including the term DFT



Application areas

IPC	**Description**	**Percentage**
H01	Basic electric elements	26%
C07	Organic chemistry	21%
C ...	Other areas of chemistry	24%
B01	Physical or chemical processes	10%
A	Health, Medical	6%
G06	Computing, Calculating, Counting	5%

Sample Atomistic and Continuum Modelling Software

	Atomistic		Continuum	
	Academic-Gov	Commercial	Academic-Gov	Commerical
Simulation Engines	VASP (EU) CASTEP (EU) Quantum Espresso (EU) Wien2k (EU) SIESTA (EU) FHI-aims (EU) Abinit (EU) Turbomole (EU) GPAW (EU) MOPAC (US) NWChem (US) Lammps(US) Gulp (US)	ATK (EU) ADF (EU) DMOL (EU) Gaussian (US) Jaguar (US)	OpenFoam Agros2D CalculiX Deal.II DUNE Elmer FEATFLOW FEATool FEAP FEB OOF (USA)	Ansys (US) Abaqus (EU) COMSOL (EU/US) ADINA Advance Design Sentaurus LS-Dyna Nastran VisualFEA (AP)
Front ends	ASE (EU) PYMATGEN (US) PyMD VMD Molden	VNL-ATK (EU) Materials Studio (EU) ADF-GUI (EU) MAPS (EU) Schrodinger (US) Gaussview (US) Culgi (EU) MEDEA (EU/US)	Paraview/VTK	Ansys (US) Abaqus (EU) COMSOL (EU/US) Sentaurus workbench (US) Simscale VisualFEA (AP) Granta (EU)

http://asdn.net/asdn/links/software.php#design

https://en.wikipedia.org/wiki/List_of_finite_element_software_packages

Commercial modelling companies

Employees	Atomistic	Continuum
<20	Scienomics (EU) Culgi (EU) Gaussian (US) SCM (EU)	Intuition software (AP)
20-100	Materials Design (EU/US) QuantumWise (EU) Schrodinger (US) Tripos (US)	Granta (EU)
100<	Dassault systems (EU)	Ansys (US) Comsol (EU/US) Synopsys (US) Dassault systems (EU)

Outline

QuantumWise

Atomic-scale modelling in the semiconductor industry

Application example: Interfaces

Concluding remarks

Company background

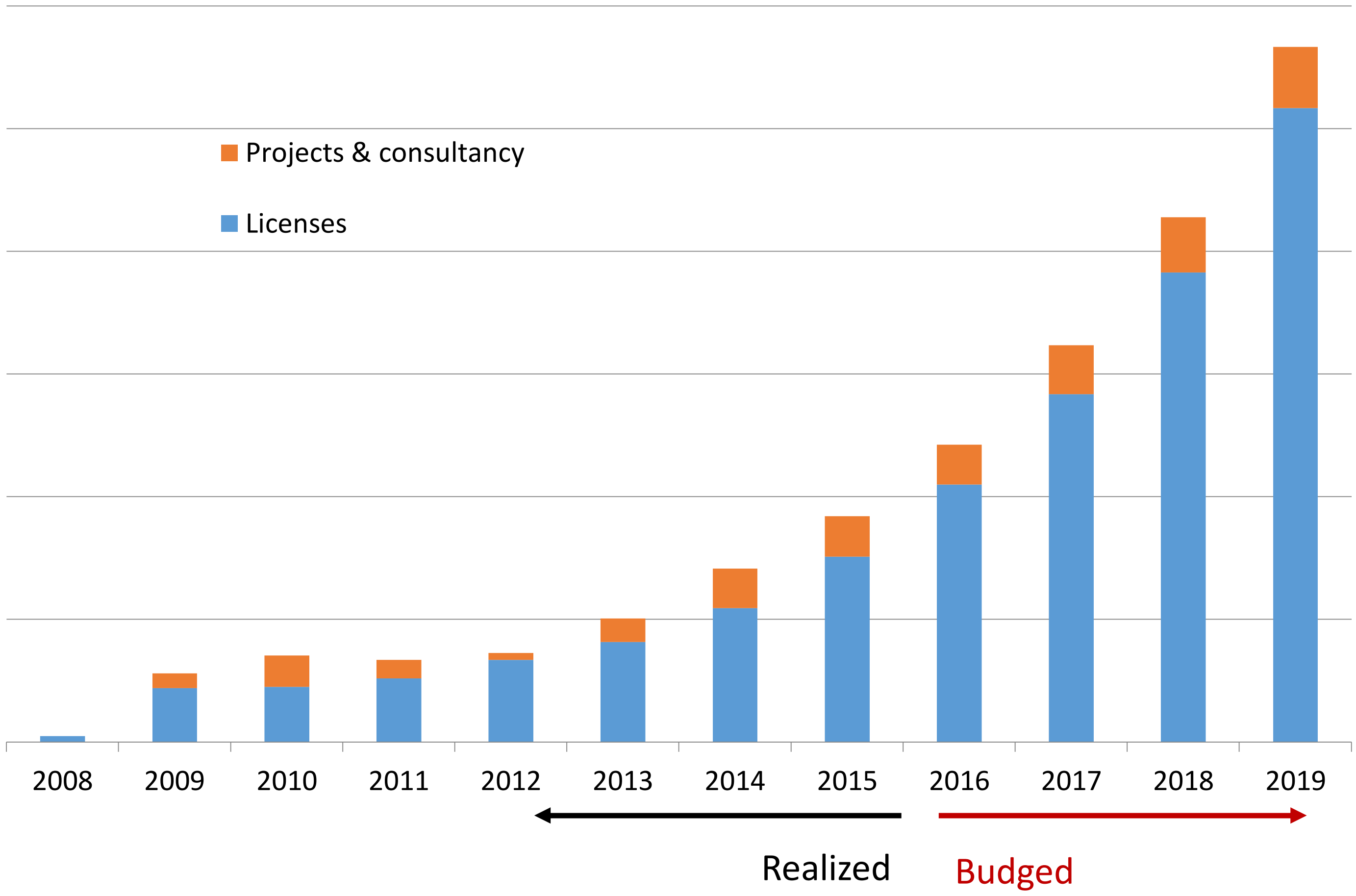
- We love science/physics - and in particular atomic scale simulations
- Help customers be more successful in atomic-scale modelling
- Internal development of quantum-mechanical simulation engines combined with community codes in certain areas
- Founded 2008, with Headquarter in Copenhagen, Denmark
- 30 FTEs; majority has a PhD (+3-5/year)
- Sales reps in USA, Singapore, Japan
- Resellers in India, China, Taiwan, Korea, …
- Profitable with 30% growth rate – no external capital

QuantumWise

BØRSEN.
GAZELLE 2015

- More than 300 users worldwide
- Rapidly expanding number of academic and industrial users

Revenue history and projections



Product offering

Nano-device simulator

Nano-device simulator with unique functionality, based on atomic-scale modeling, which can replace/complement current TCAD device simulators that use a continuum description

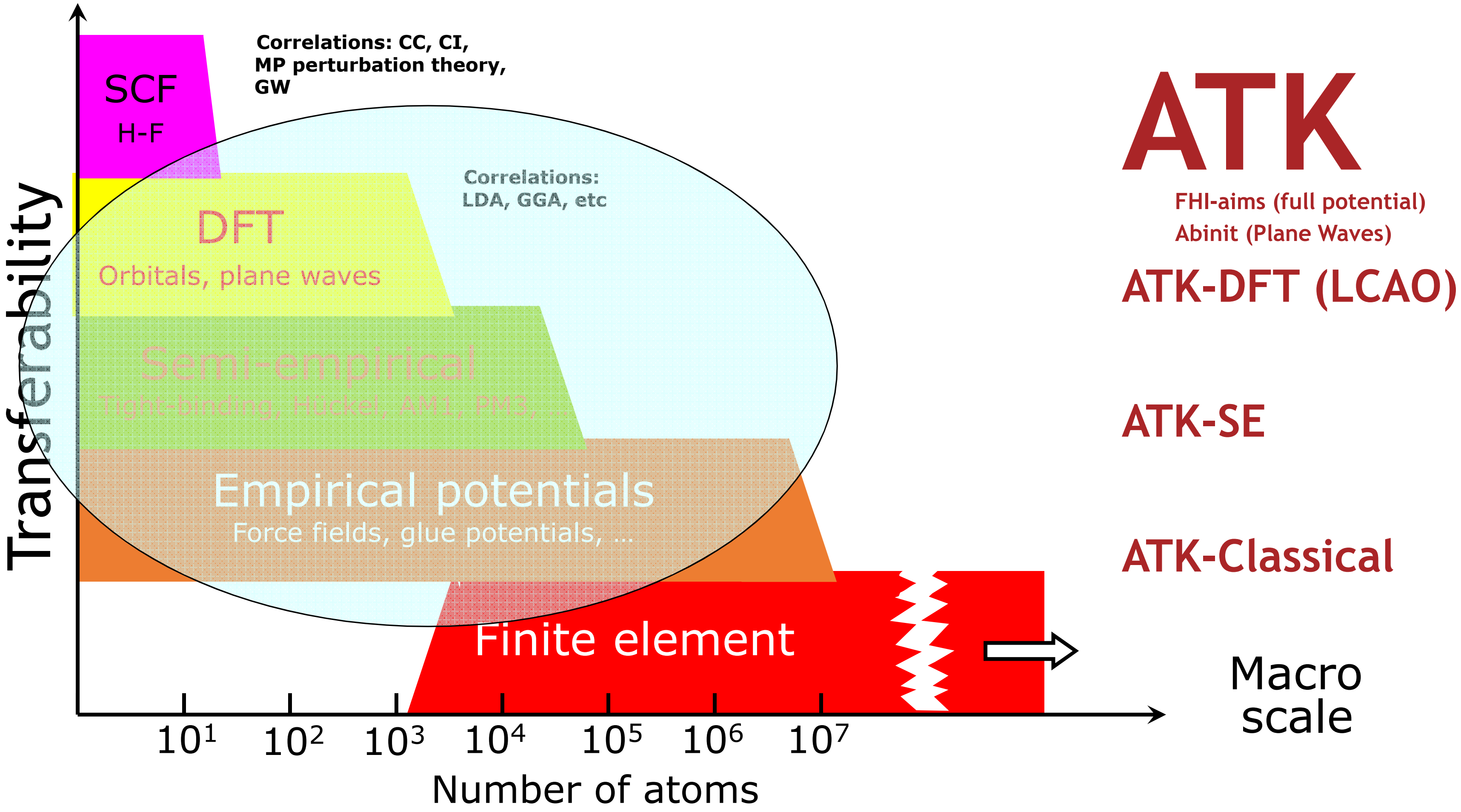
- Simulation of semiconductor, magnetic and interface systems
- Other emerging devices, molecular electronics, organic crystals

Atomic-scale modeling platform

Professional platform which integrates multiple atomic-scale modeling techniques, that can accelerate R&D within materials and electronics in multiple industry sectors

- Fast and accurate DFT calculations + semiempirical models
- Interface to other simulation engines (like VASP, Abinit, FHIaims, QuantumEspresso, GPAW, SIESTA, Wien2k)
- Industry-quality classical MD engine
- Calculation of parameters for TCAD tools

Atomistix ToolKit (ATK)



ATK

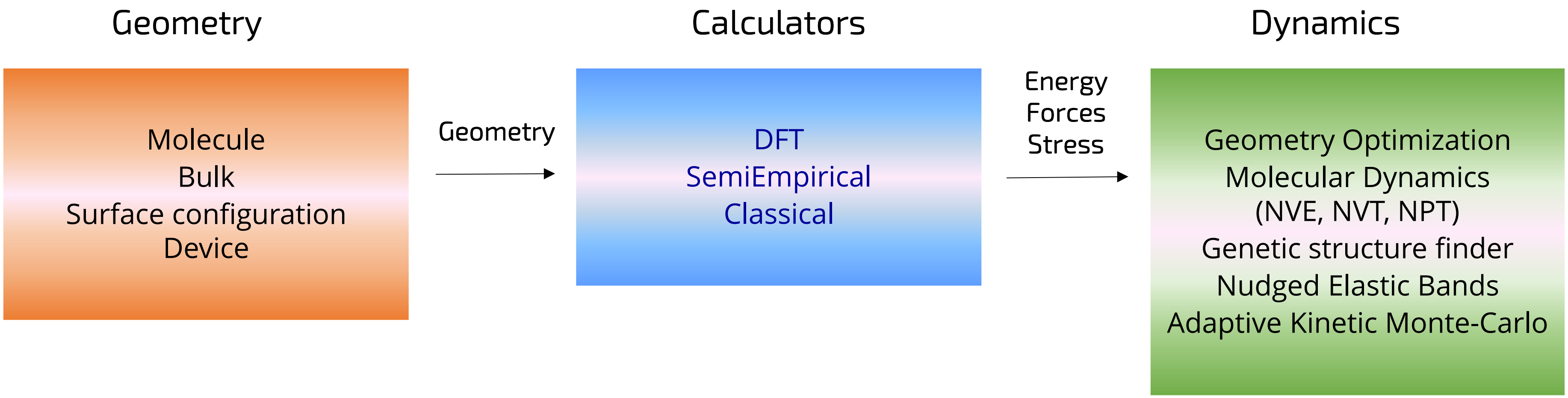
FHI-aims (full potential)
Abinit (Plane Waves)

ATK-DFT (LCAO)

ATK-SE

ATK-Classical

Python interface to atomic-scale simulations



Geometry

Molecule
Bulk
Surface configuration
Device

Geometry →

Calculators

DFT
SemiEmpirical
Classical

Energy
Forces
Stress →

Dynamics

Geometry Optimization
Molecular Dynamics
(NVE, NVT, NPT)
Genetic structure finder
Nudged Elastic Bands
Adaptive Kinetic Monte-Carlo

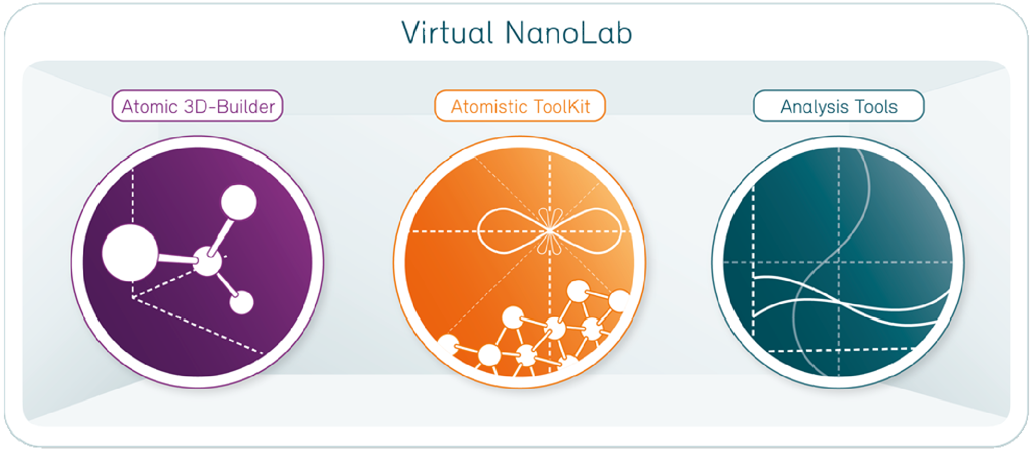
Band structure
DOS
Complex band structure
Effective band structure
Effective mass
Piezoelectric properties
Optical properties
ELF
Bloch states
Total energy
Electron density
Potential

Forces, stress
Local stress/atoms
Dynamical matrix
Elastic constants
Phonon spectrum/DOS

Deformation potential
Mobility
Inelastic current

Transmission spectrum
I-V curve
Local/device DOS
Transmission eigenstates
Transmission pathways
Current density
Spin transfer torque

Virtual NanoLab with the Atomistix ToolKit (ATK)



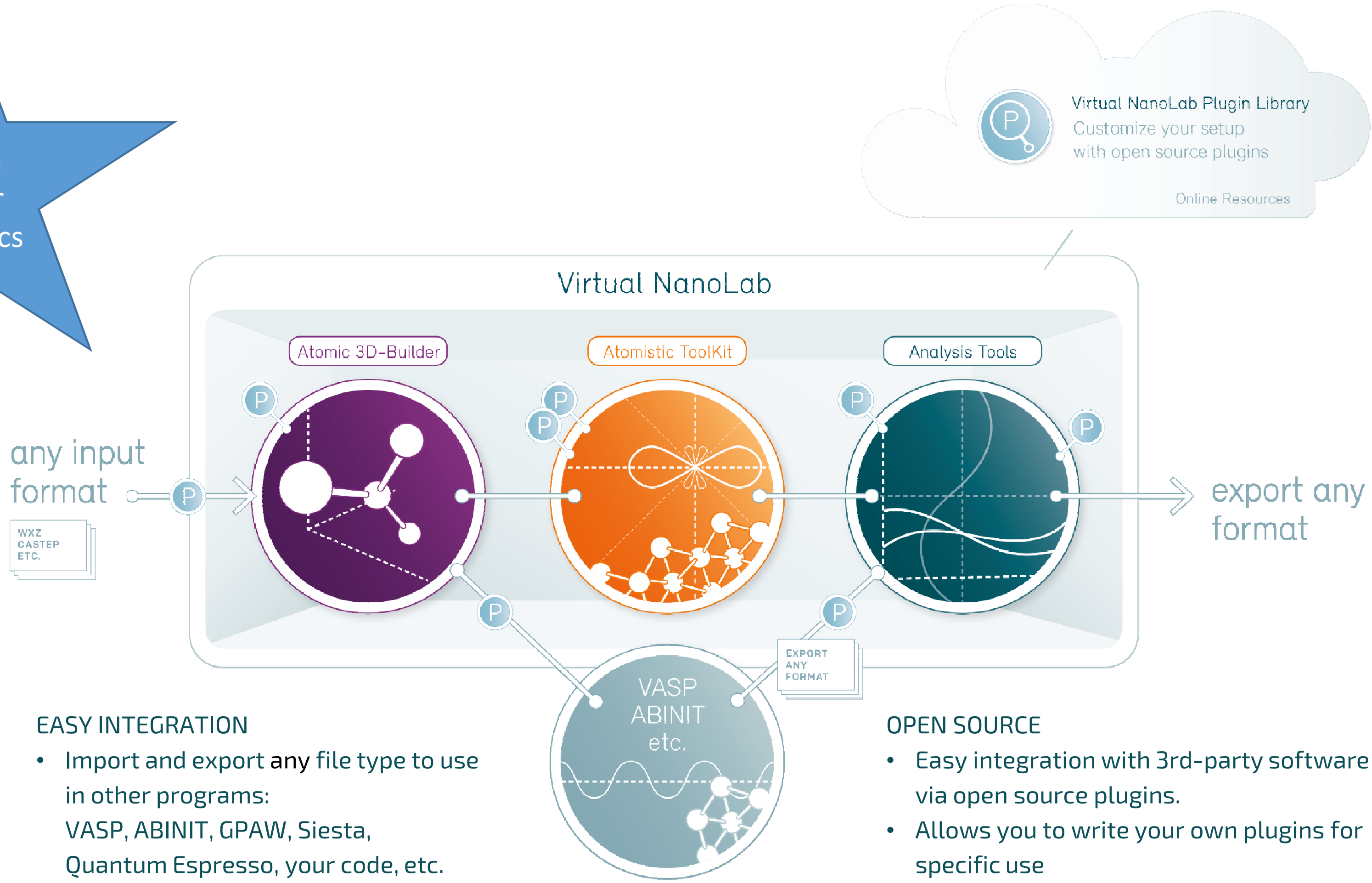
Build
Interfaces
Nanotubes
Nanosheets
Nanopribbons
Molecules
Crystals by symmetry
Cleave surfaces
Polycrystals

Methods
DFT
Semi-Empirical
Classical potentials
(Abinit)
(FHI-Aims)
Non-Equilibrium Green's Functions (NEGF) formalism

Analyze results
3D visualizations, isosurfaces
Manipulate 3D grids
Band structure, density of states
MD trajectory analysis
Analyze and visualize your data
Produce movies and animated GIFs

Virtual NanoLab, GUI for ATK and other simulators

Base
version
free for
academics



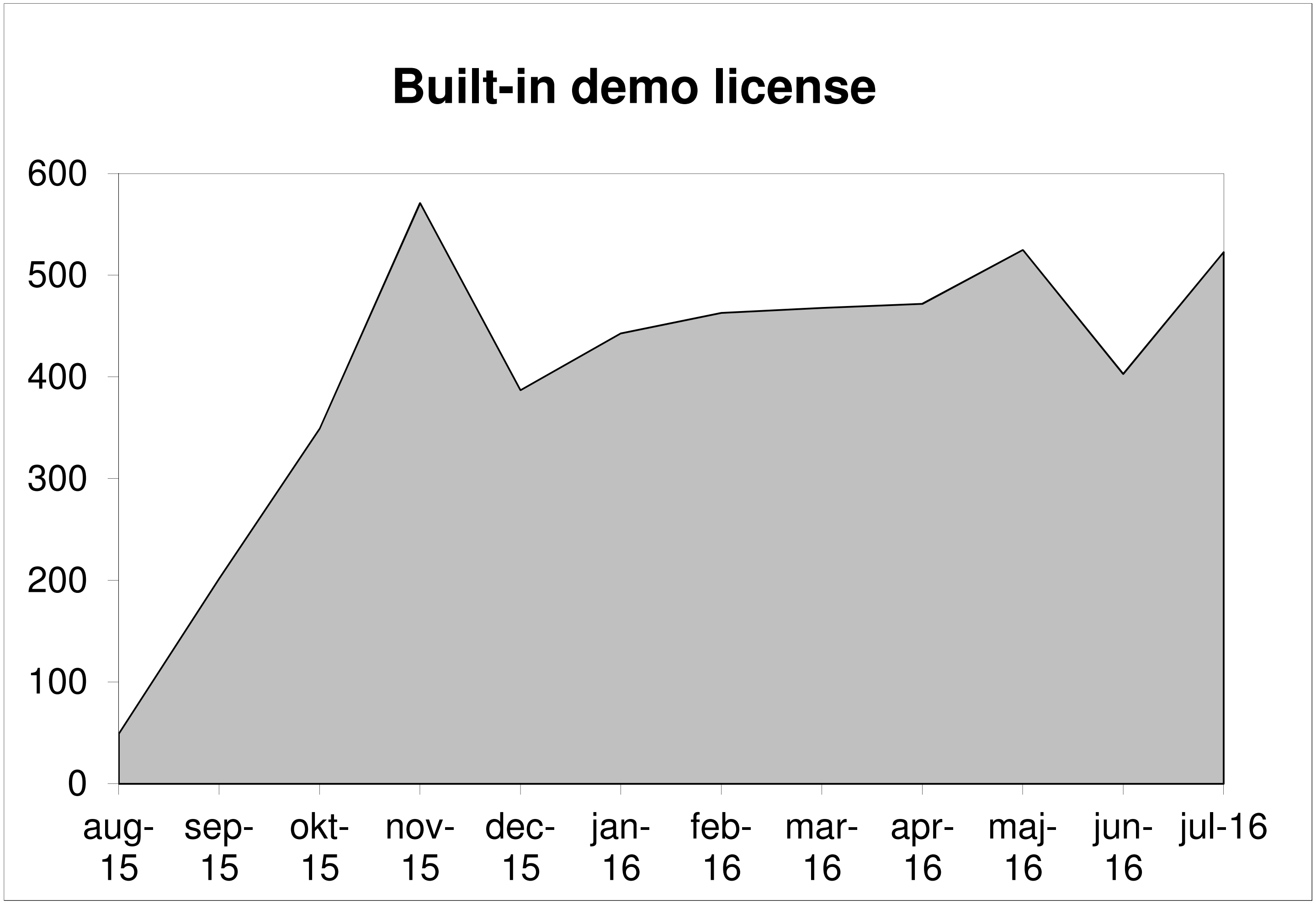
EASY INTEGRATION

- Import and export any file type to use in other programs:
  VASP, ABINIT, GPAW, Siesta, Quantum Espresso, your code, etc.

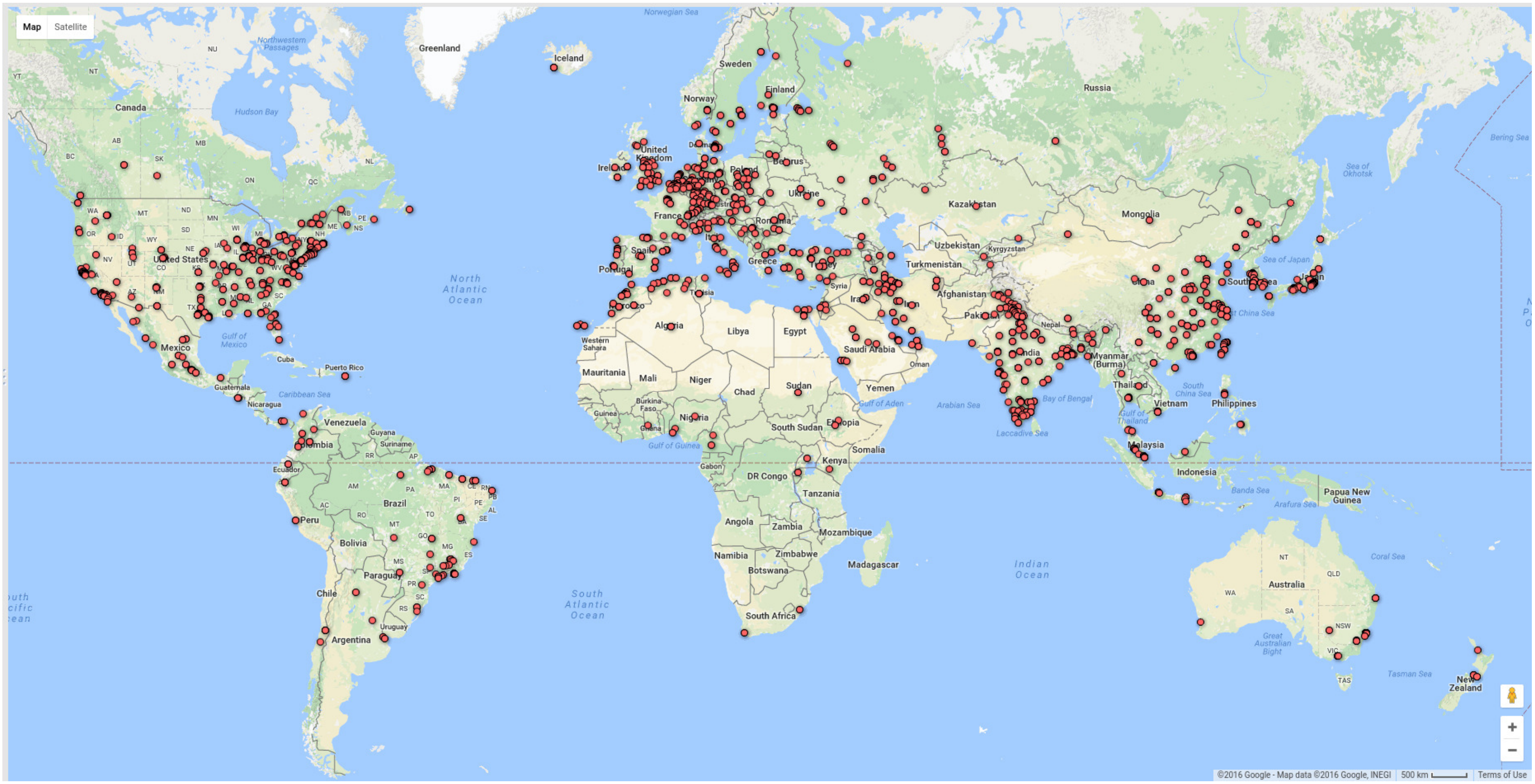
OPEN SOURCE

- Easy integration with 3rd-party software via open source plugins.
- Allows you to write your own plugins for specific use

Activation of VNL/ATK license



World users


Map
Satellite
Greenland
Iceland
Canada
Hudson Bay
Northwestern Passages
United States
Mexico
Gulf of Mexico
Cuba
Puerto Rico
Guatemala
Nicaragua
Caribbean Sea
Venezuela
Colombia
Guyana
Suriname
Ecuador
Peru
Brazil
Bolivia
Paraguay
Chile
Argentina
Uruguay
North Atlantic Ocean
South Atlantic Ocean
Norwegian Sea
Sweden
Norway
Finland
Russia
Ireland
United Kingdom
Denmark
Poland
Belarus
Ukraine
France
Spain
Portugal
Romania
Greece
Kazakhstan
Mongolia
Uzbekistan
Kyrgyzstan
Turkmenistan
Afghanistan
Pakistan
Iran
Iraq
Syria
Tunisia
Algeria
Libya
Egypt
Western Sahara
Mauritania
Mali
Niger
Chad
Sudan
South Sudan
Ethiopia
Somalia
Kenya
Burkina Faso
Guinea
Ghana
Nigeria
Gulf of Guinea
Gabon
DR Congo
Tanzania
Angola
Zambia
Mozambique
Namibia
Zimbabwe
Botswana
Madagascar
South Africa
Saudi Arabia
Oman
Yemen
Gulf of Aden
Arabian Sea
Laccadive Sea
India
Nepal
Bay of Bengal
Myanmar (Burma)
Thailand
Gulf of Thailand
Vietnam
South China Sea
Philippines
Malaysia
Indonesia
China
South Korea
Japan
Sea of Japan
East China Sea
Sea of Okhotsk
Bering Sea
Banda Sea
Arafura Sea
Papua New Guinea
Coral Sea
Indian Ocean
Australia
Great Australian Bight
Tasman Sea
New Zealand
South Pacific Ocean
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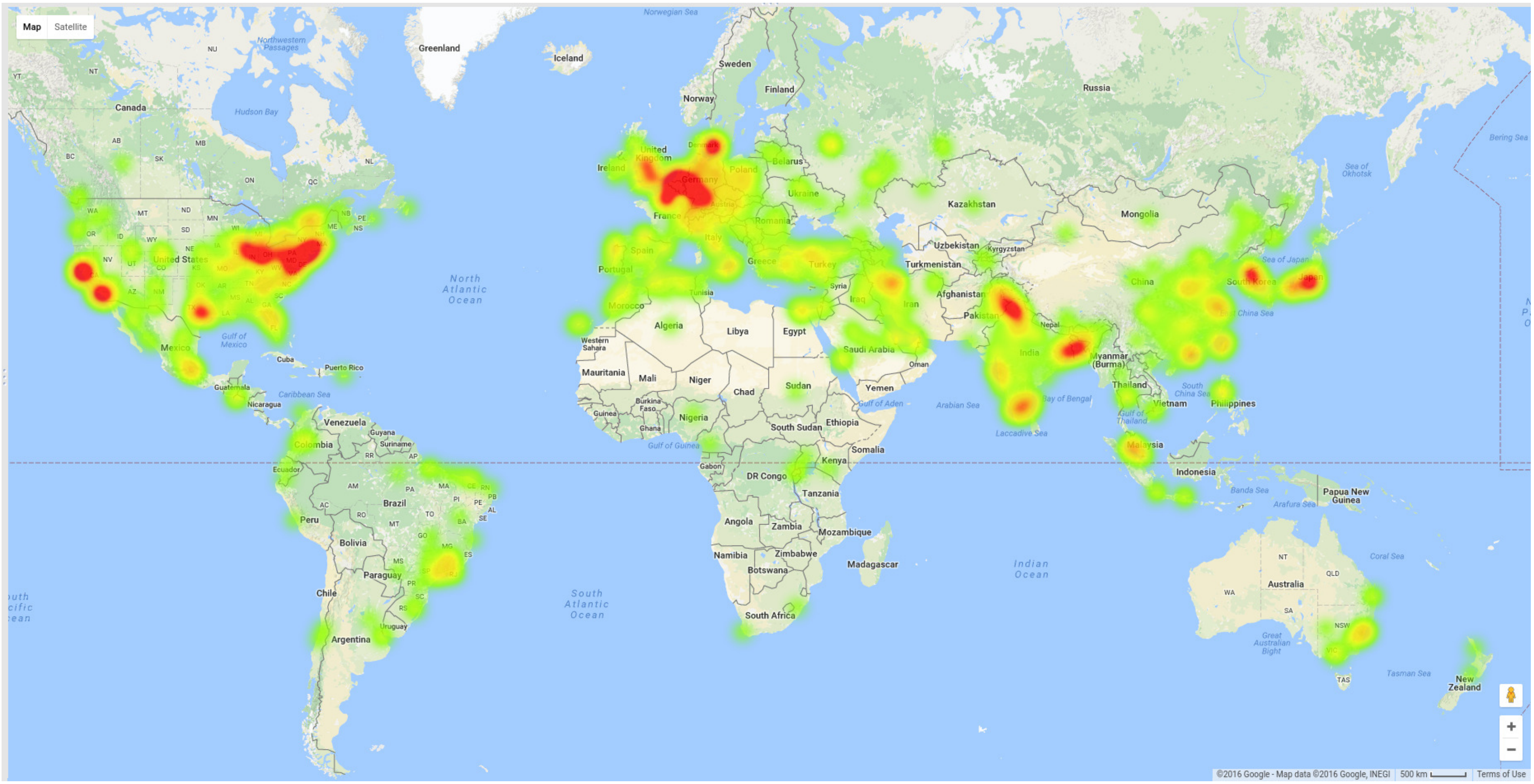
500 km
Terms of Use

World users


Map
Satellite
Norwegian Sea
Greenland
Iceland
Sweden
Finland
Norway
Russia
Northwestern Passages
NU
NT
YT
Canada
Hudson Bay
AB
MB
BC
SK
ON
QC
NL
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PE
NS
ME
WA
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ND
MN
OR
ID
SD
WY
NE
NV
UT
United States
CO
KS
MO
AZ
NM
OK
AR
TX
LA
MS
AL
GA
FL
Gulf of Mexico
Mexico
Cuba
Puerto Rico
Guatemala
Caribbean Sea
Nicaragua
Venezuela
Guyana
Suriname
Colombia
Ecuador
Peru
Brazil
Bolivia
Paraguay
Chile
Argentina
Uruguay
North Atlantic Ocean
South Atlantic Ocean
Ireland
United Kingdom
Denmark
Belarus
Poland
Germany
Ukraine
France
Austria
Romania
Italy
Spain
Portugal
Greece
Turkey
Morocco
Tunisia
Algeria
Libya
Egypt
Western Sahara
Mauritania
Mali
Niger
Chad
Sudan
Nigeria
Burkina Faso
Guinea
Ghana
Gulf of Guinea
South Sudan
Ethiopia
Somalia
Kenya
Gabon
DR Congo
Tanzania
Angola
Zambia
Mozambique
Namibia
Zimbabwe
Botswana
Madagascar
South Africa
Saudi Arabia
Oman
Yemen
Gulf of Aden
Syria
Iraq
Iran
Kazakhstan
Uzbekistan
Kyrgyzstan
Turkmenistan
Afghanistan
Pakistan
Nepal
India
Arabian Sea
Laccadive Sea
Bay of Bengal
Myanmar (Burma)
Thailand
Gulf of Thailand
Vietnam
South China Sea
Philippines
Malaysia
Indonesia
Mongolia
China
South Korea
Japan
Sea of Japan
East China Sea
Sea of Okhotsk
Bering Sea
Banda Sea
Arafura Sea
Papua New Guinea
Coral Sea
Indian Ocean
Australia
NT
QLD
WA
SA
NSW
VIC
TAS
Great Australian Bight
Tasman Sea
New Zealand
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500 km
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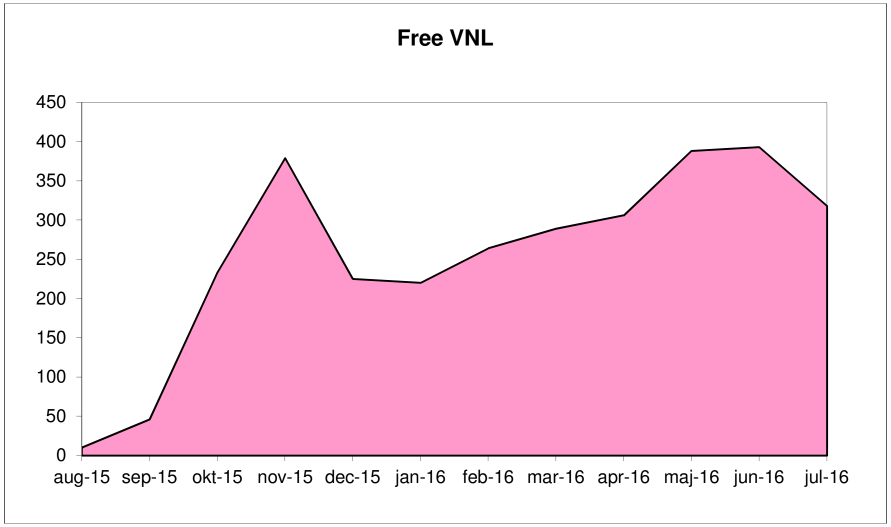
Free VNL users



Total licenses sent: 3307
Unique users: 2568
(each account can request up to three licenses)

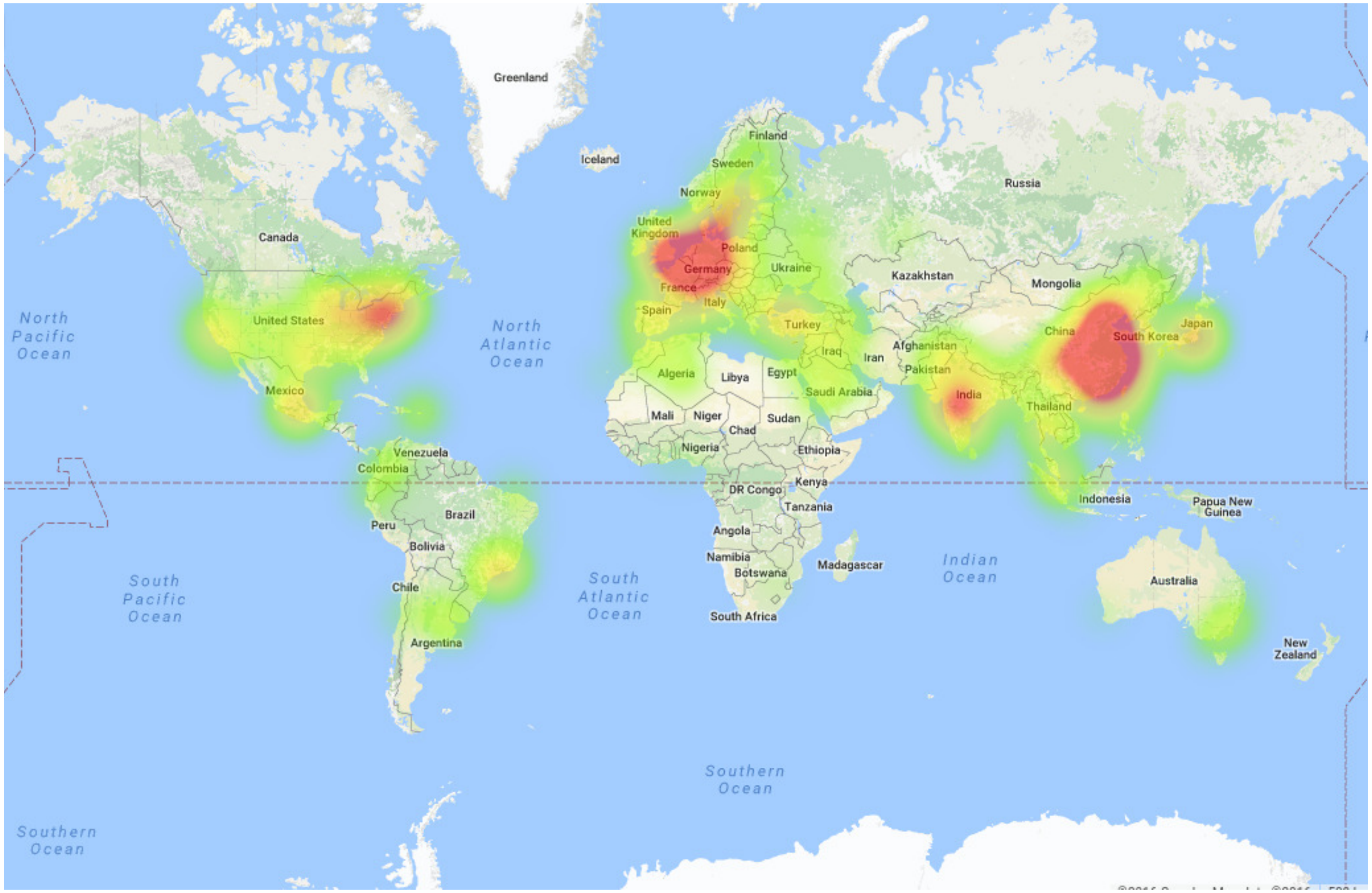
From 90 different countries

Top 10 countries:

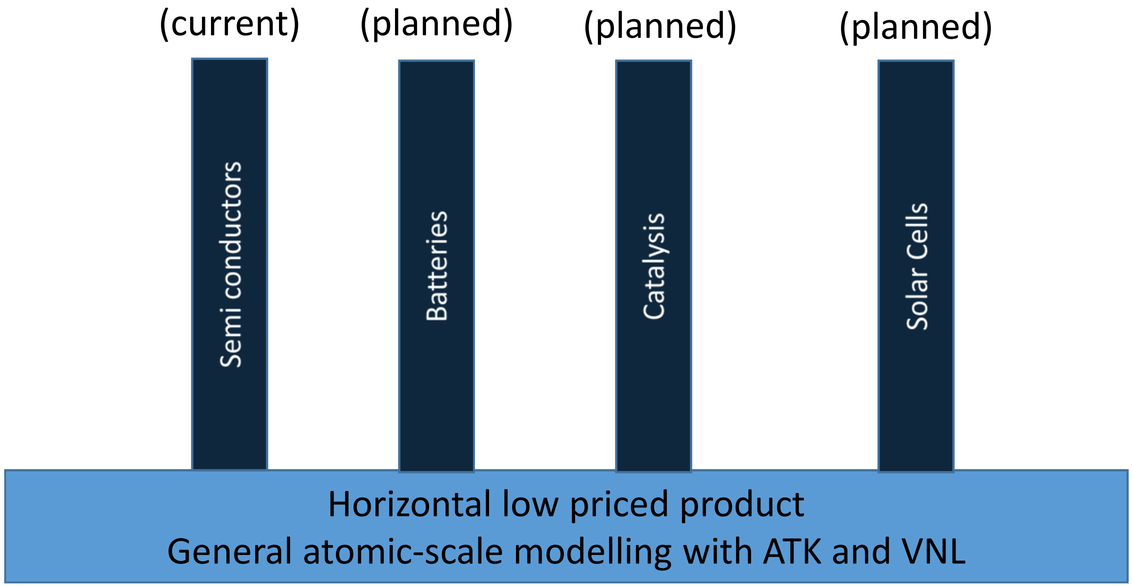
705	China
536	United States
373	India
122	Germany
112	Japan
108	Brazil
97	United Kingdom
81	Korea
79	Mexico
60	Spain

Map of free VNL users

Map of free VNL users



Overall product strategy



(current)

Semi conductors

(planned)

Batteries

(planned)

Catalysis

(planned)

Solar Cells

Horizontal low priced product
General atomic-scale modelling with ATK and VNL

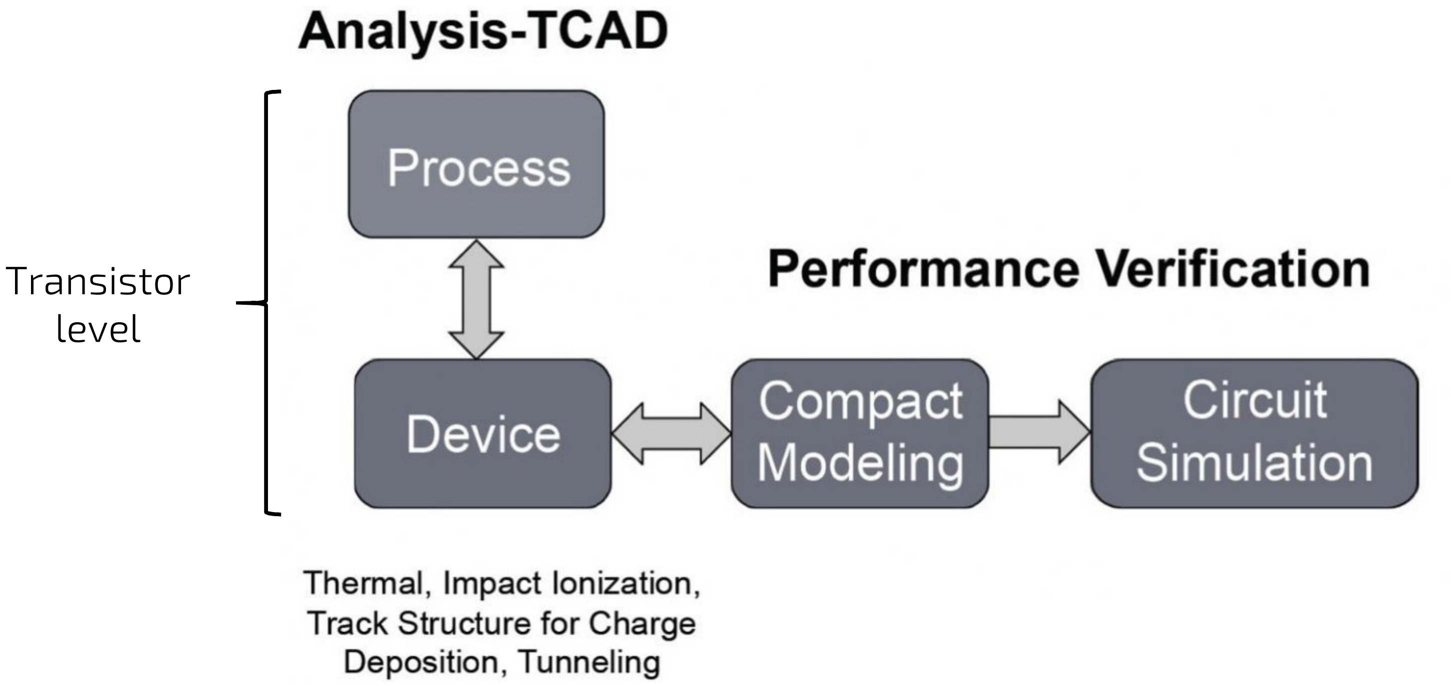
Outline

- QuantumWise
- **Atomic-scale modelling in the semiconductor industry**
- Application example: Interfaces
- Concluding remarks

Atomic-scale modelling in the semiconductor industry

Simulation an integral part of the semiconductor industry

The simulation software is develop by the Electronic Design Automation (EDA) software industry



Analysis-TCAD

Performance Verification

Process

Device

Compact Modeling

Circuit Simulation

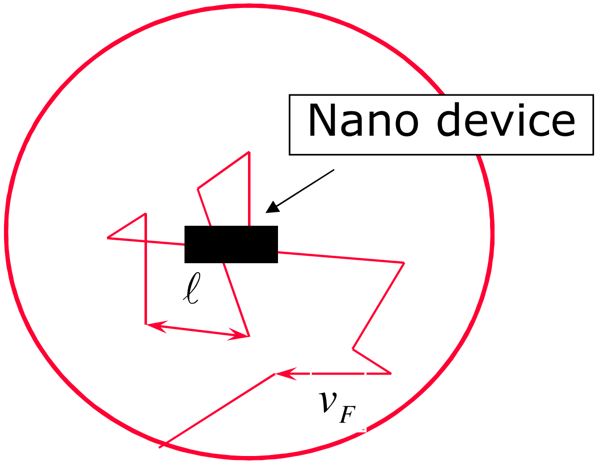
Transistor level

Thermal, Impact Ionization, Track Structure for Charge Deposition, Tunneling

Current TCAD tools use drift-diffusion

Electrons move around randomly
with some average velocity

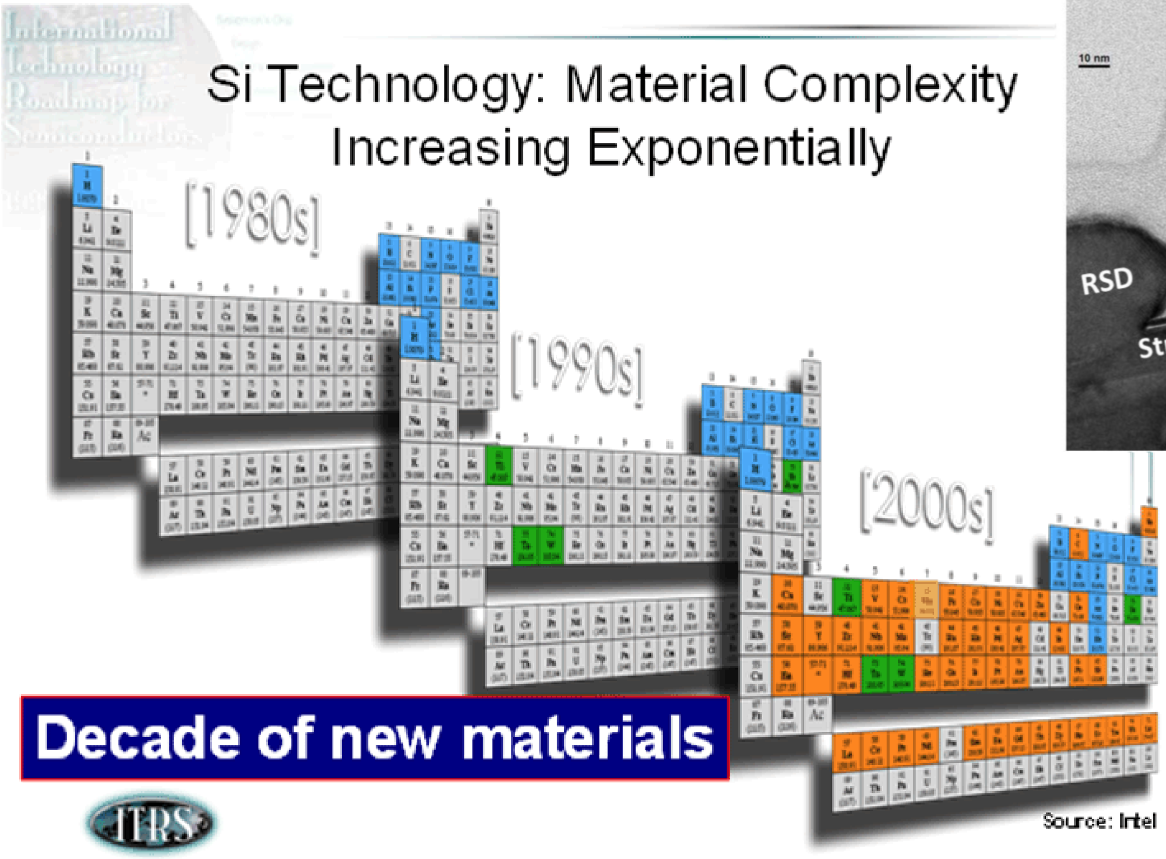
$$v_F = \langle \vec{v}_0 \rangle$$

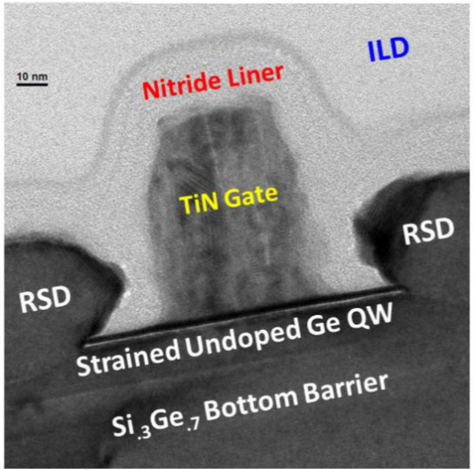

Nano device

This picture breaks down when the device dimensions are smaller than the mean free path l

Furthermore, difficult to generate parameters for the simulation models

Nano means new materials





Ge p-channel quantum well field-effect transistor (QWFET) presented by Intel at IEDM 2010

Atomic-scale modelling in the semiconductor industry

1. Calculate materials parameters that can be part of multi-scale workflow
    - Defect formation energies, diffusion lengths
    - band structure of confined systems
    - band offsets at interfaces
    - Emerging devices, graphene, spintronics, …

2. Perform device modelling at the quantum level for benchmarking continuum level models
    - FINFET's
    - p-i-n junctions

Outline

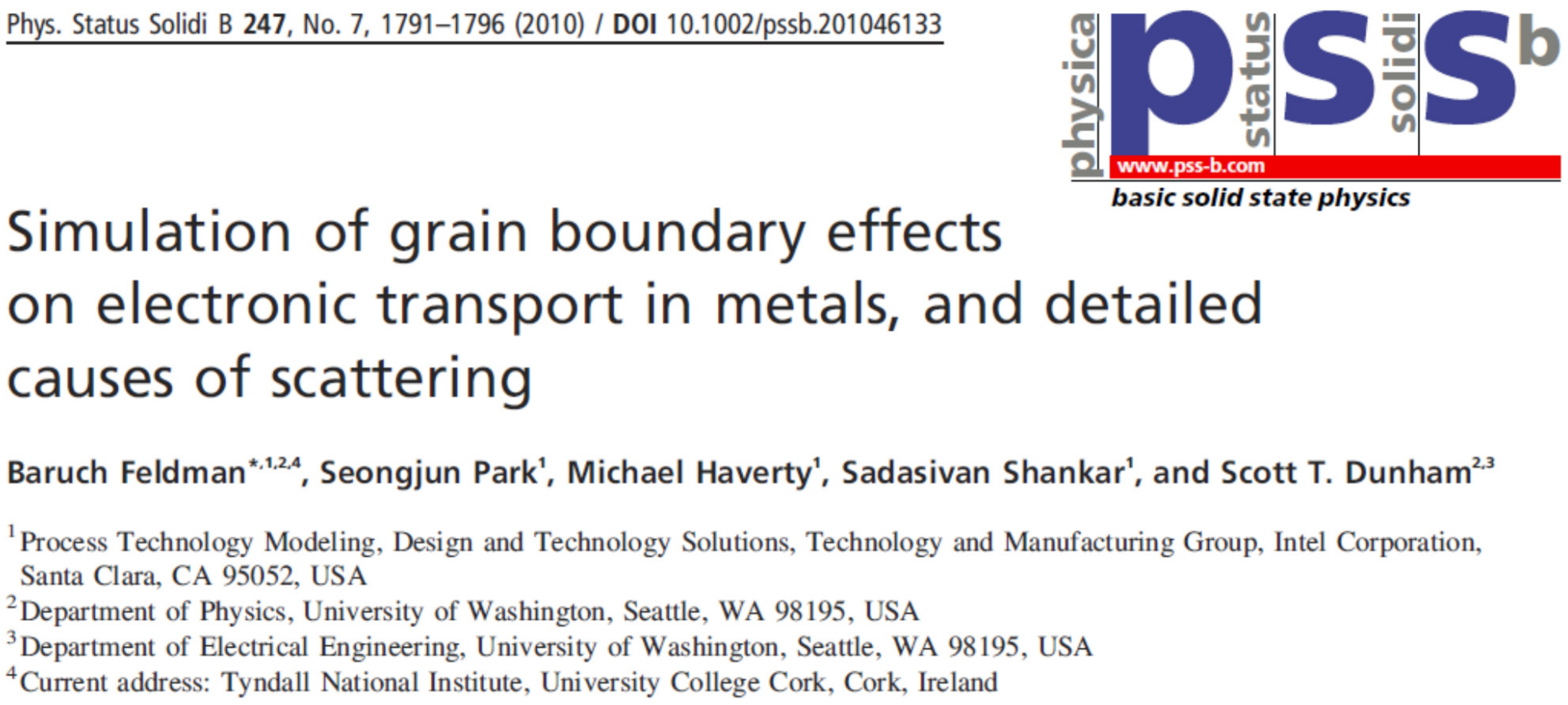
QuantumWise

Atomic-scale modelling in the semiconductor industry

Application example: Interfaces

Concluding remarks

Simulation of transport across grain boundaries



Phys. Status Solidi B **247**, No. 7, 1791–1796 (2010) / **DOI** 10.1002/pssb.201046133

physica status solidi pss b
www.pss-b.com
basic solid state physics

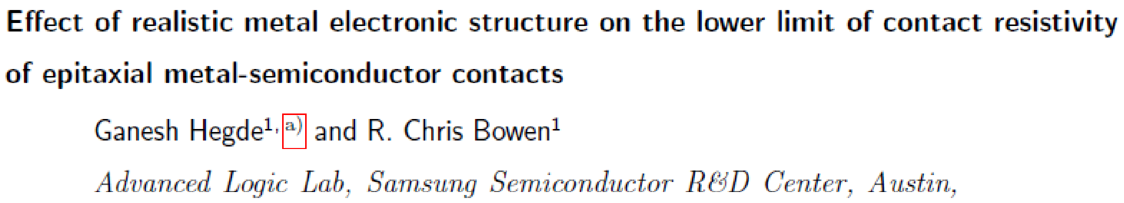
Simulation of grain boundary effects on electronic transport in metals, and detailed causes of scattering

Baruch Feldman[*,1,2,4], **Seongjun Park**[1], **Michael Haverty**[1], **Sadasivan Shankar**[1], **and Scott T. Dunham**[2,3]

[1] Process Technology Modeling, Design and Technology Solutions, Technology and Manufacturing Group, Intel Corporation, Santa Clara, CA 95052, USA
[2] Department of Physics, University of Washington, Seattle, WA 98195, USA
[3] Department of Electrical Engineering, University of Washington, Seattle, WA 98195, USA
[4] Current address: Tyndall National Institute, University College Cork, Cork, Ireland

Simulation of metal-semiconductor interface

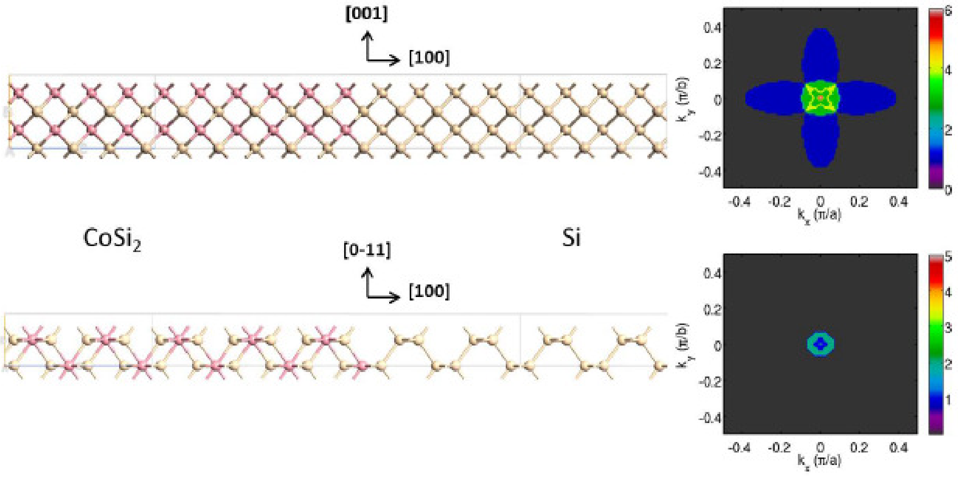
Arxiv:1405.1317v1 [cond-mat.mtrl-sci]



Effect of realistic metal electronic structure on the lower limit of contact resistivity of epitaxial metal-semiconductor contacts

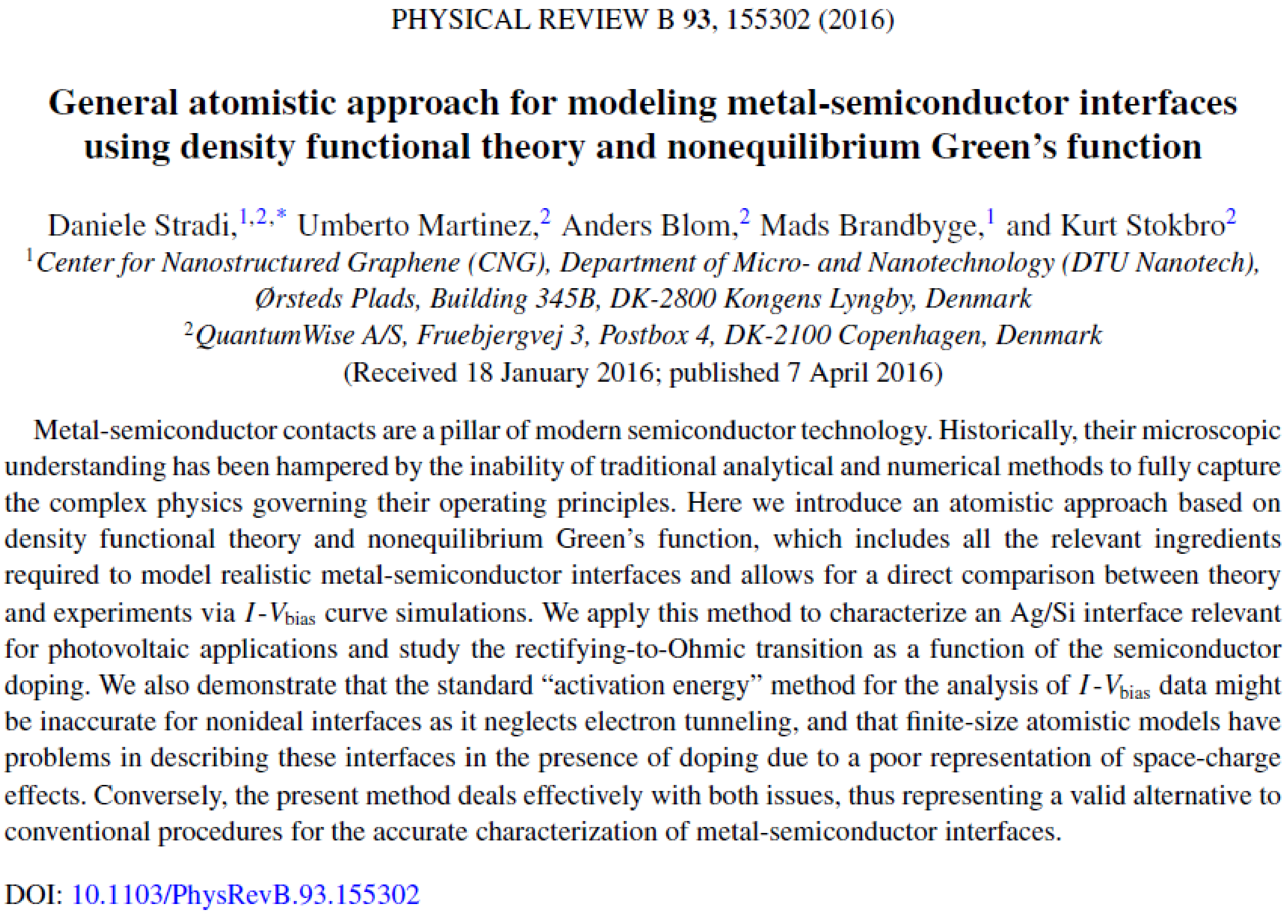
Ganesh Hegde[1, a)] and R. Chris Bowen[1]

Advanced Logic Lab, Samsung Semiconductor R&D Center, Austin,



“Valley filtering”

Methodology described in recent PRB paper



PHYSICAL REVIEW B **93**, 155302 (2016)

General atomistic approach for modeling metal-semiconductor interfaces using density functional theory and nonequilibrium Green's function

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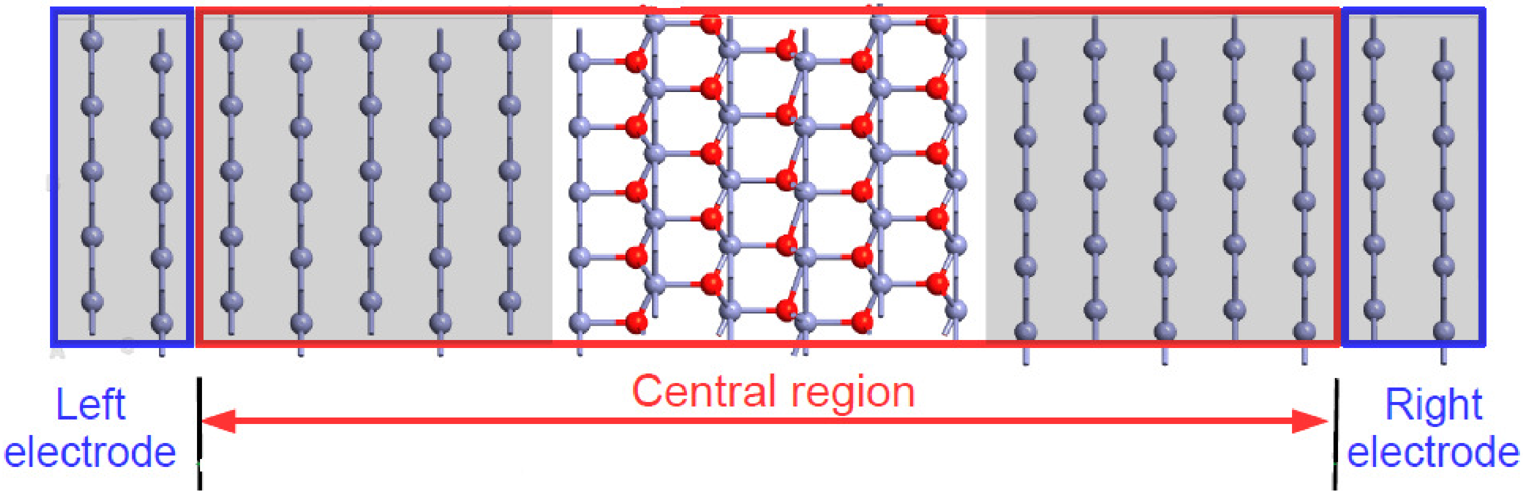
Metal-semiconductor contacts are a pillar of modern semiconductor technology. Historically, their microscopic understanding has been hampered by the inability of traditional analytical and numerical methods to fully capture the complex physics governing their operating principles. Here we introduce an atomistic approach based on density functional theory and nonequilibrium Green's function, which includes all the relevant ingredients required to model realistic metal-semiconductor interfaces and allows for a direct comparison between theory and experiments via I-V_{bias} curve simulations. We apply this method to characterize an Ag/Si interface relevant for photovoltaic applications and study the rectifying-to-Ohmic transition as a function of the semiconductor doping. We also demonstrate that the standard "activation energy" method for the analysis of I-V_{bias} data might be inaccurate for nonideal interfaces as it neglects electron tunneling, and that finite-size atomistic models have problems in describing these interfaces in the presence of doping due to a poor representation of space-charge effects. Conversely, the present method deals effectively with both issues, thus representing a valid alternative to conventional procedures for the accurate characterization of metal-semiconductor interfaces.

DOI: 10.1103/PhysRevB.93.155302

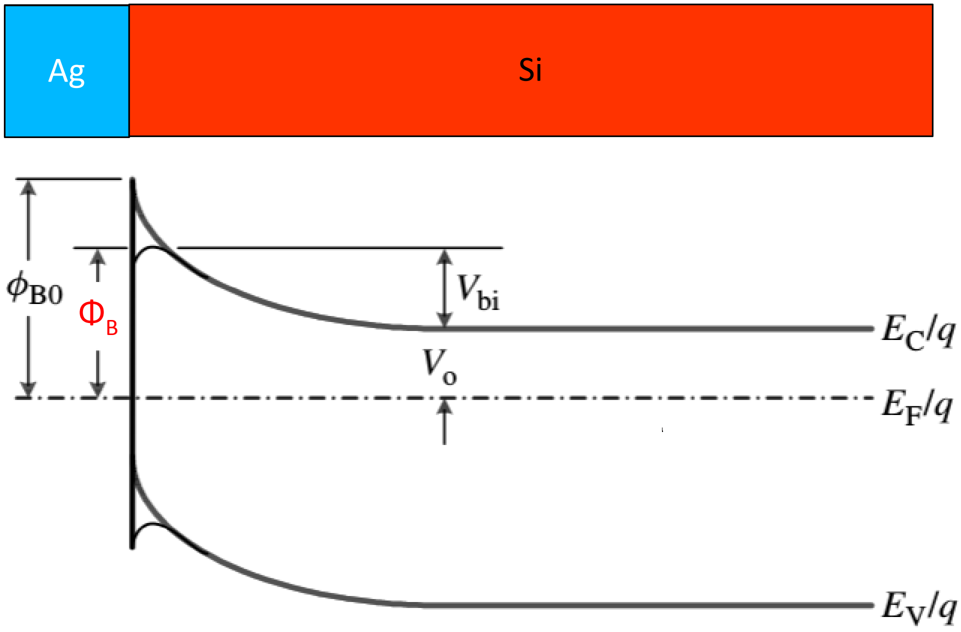
NEGF transport methodology



- The system is divided into 3 regions: left, central, right regions
- Properties of left and right regions are calculated using PBC
- The electron density of the central region is donated by the electrode reservoirs, i.e. open boundary conditions
- The electro-static potential of the central region is obtained from the density and using the electrode boundary conditions

M. Brandbyge et. al. PRB. ***65****, 165401 (2002). Stradi et. al. PRB 93, 155302 (2016).*

Metal-Semiconductor Schottky contact



Φ_{B0}= Ideal barrier height
Φ_B = Effective barrier height
V_{bi} = build in potential
V_0 = potential (E_F-E_V)

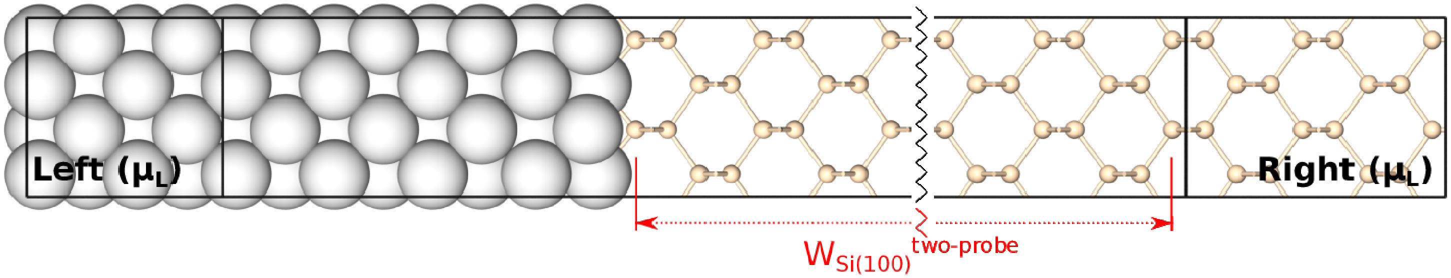
In the thermionic regime the current is described by:

$$I = AA' T^2 e^{-q\Phi_B/k_BT}\left(e^{qV/nk_BT} - 1\right)$$

I = current
A' = $4\pi qk^2m^*/h^3$ (Richardson constant)
A = electrically active area
n = ideality factor

*Sze, Ng *Physics of Semiconductor Interfaces 3rd ed.* Wiley 2007
Schroeder *Semiconductor Material and Device Characterization 3rd ed.* Wiley 2006

Model Ag(100)/Si(100) investigated using DFT+NEGF

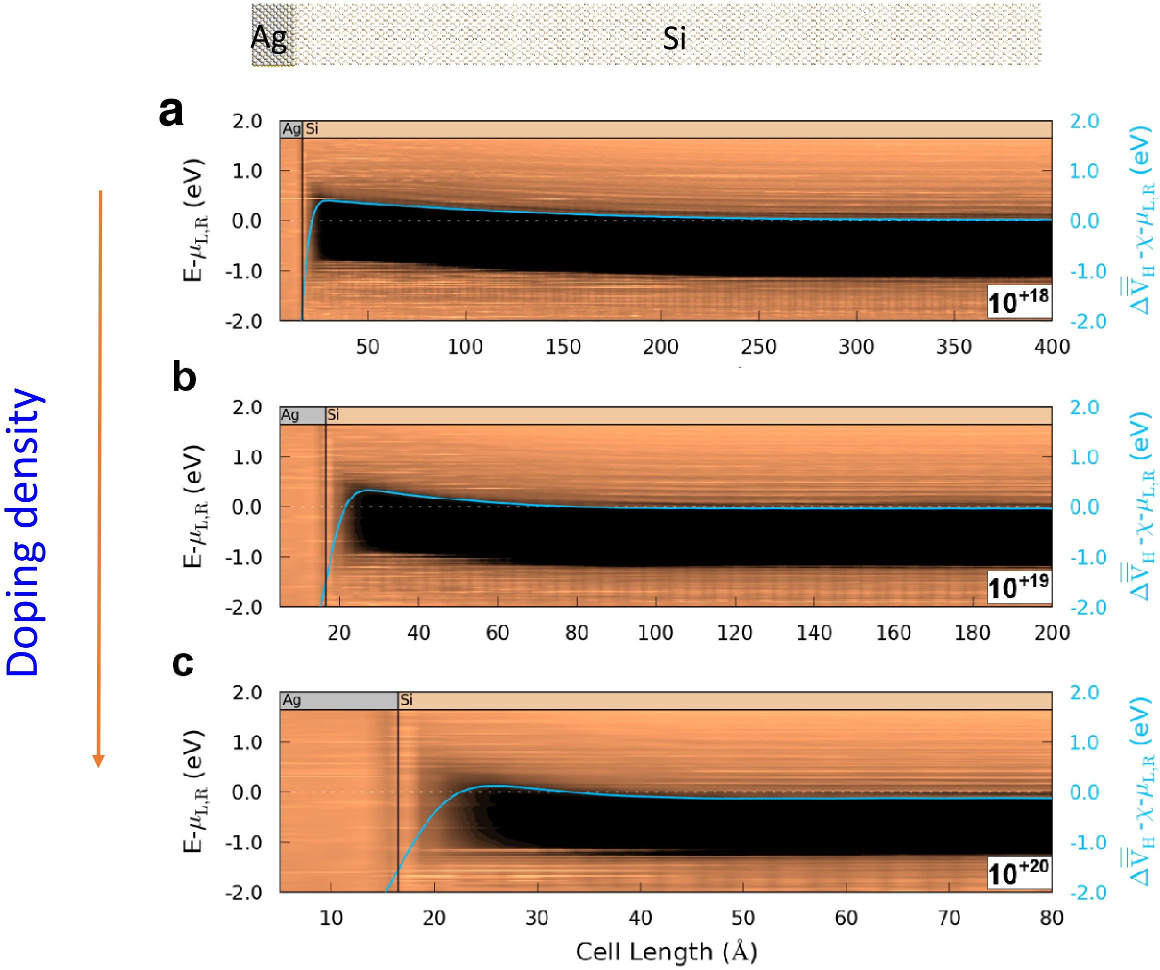


- **DFT+NEGF formalism***: exact representation of the non-periodic interface
- **Meta-GGA functional****: correctly accounts for the silicon band gap (E_g = 1.17 eV)
- **Effective doping** of the silicon side using localized charges on the Si atoms

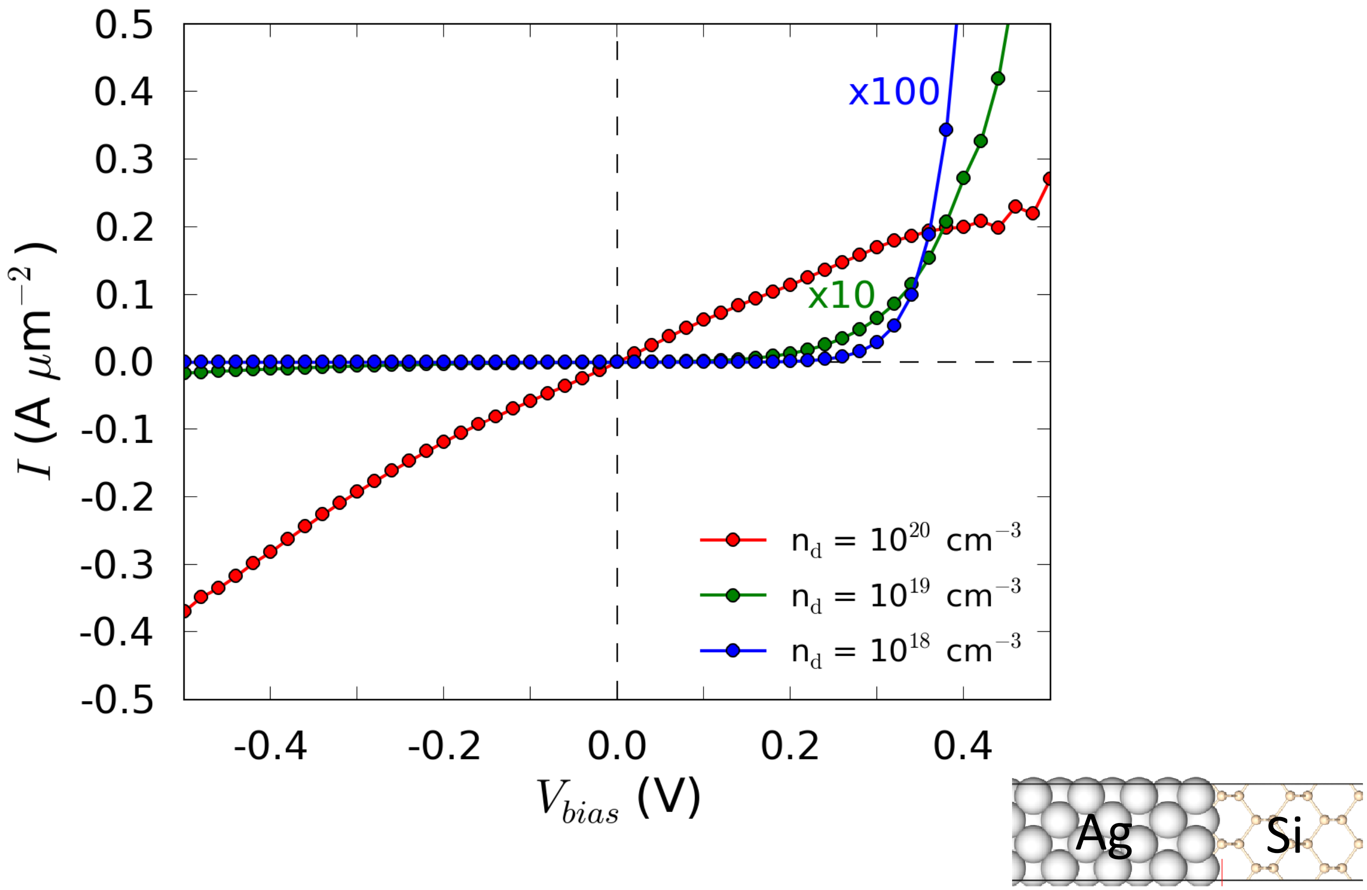
Stradi et. al. *Phys. Rev. B* **93**, 155302 (2016).

*Brandbyge et al. *Phys. Rev. B* **65**, 165401 (2002)
** Tran, Blaha *Phys. Rev. Lett.***102**, 226401 (2009)

Band bending as function of doping



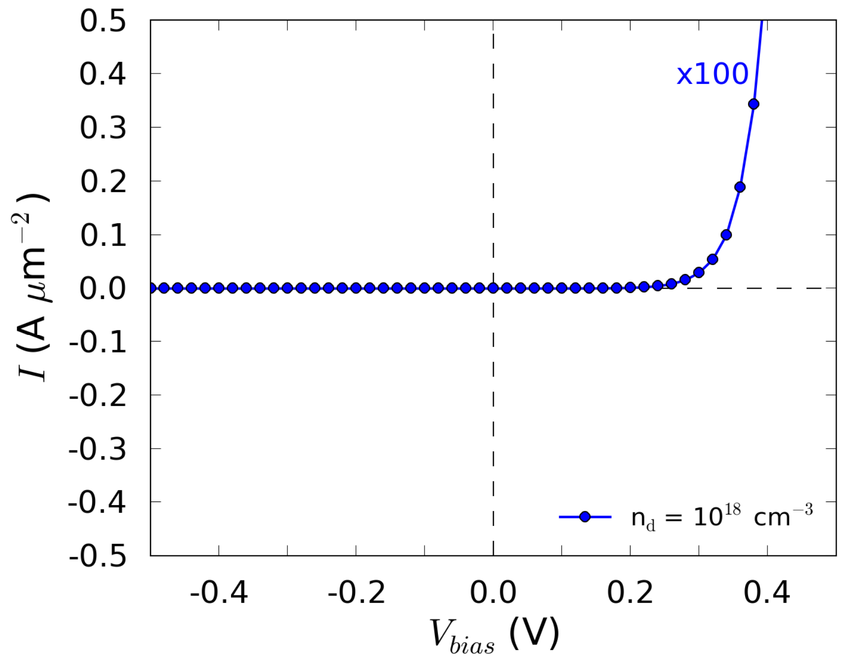
Calculated I-V characteristics

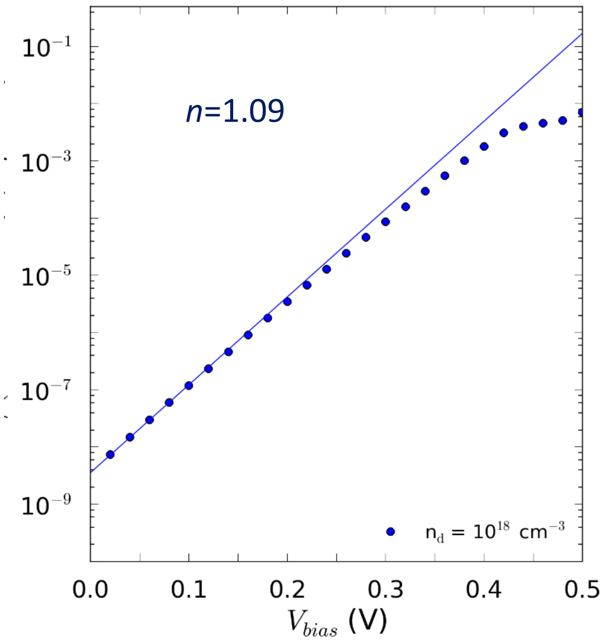


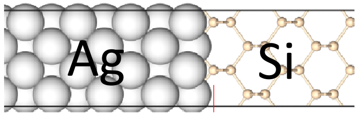
Calculated I-V characteristics and extraction of ideality factor n

$$I = AA' \, T^2 e^{-q\Phi_B / k_B T}\left(e^{qV / n k_B T} - 1\right)$$

$$I = I_0\left(e^{qV / n k_B T} - 1\right)$$

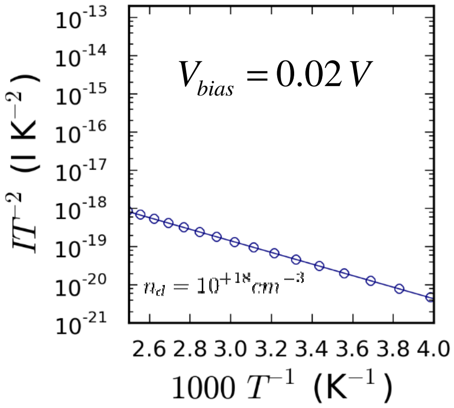


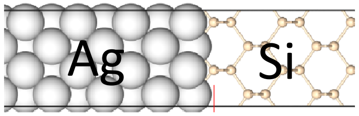




Schottky barrier from temperature dependence

$$I = AA' \, T^2 e^{-q\Phi_B/k_BT}\left(e^{qV/nk_BT} - 1\right) \Rightarrow -\frac{k_B}{q}\frac{d[\ln(I/T^2)]}{d(1/T)} = \Phi^{\mathrm{AE}} - \frac{V_{bias}}{n}$$





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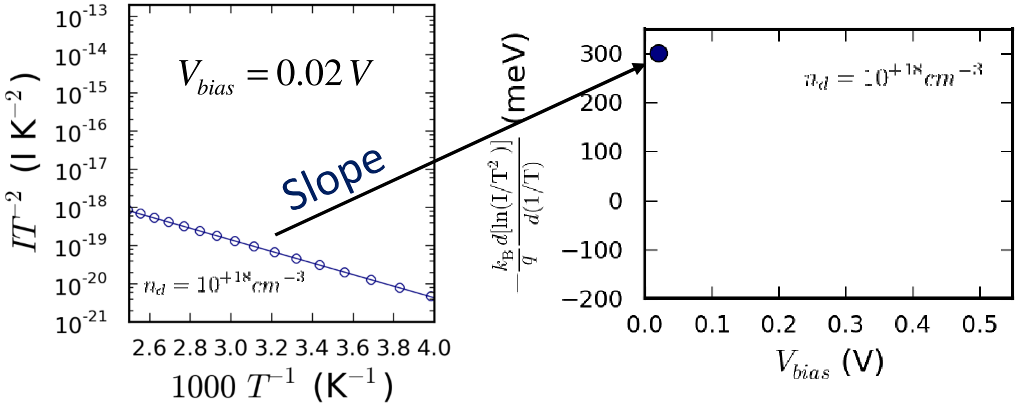
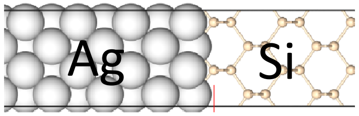
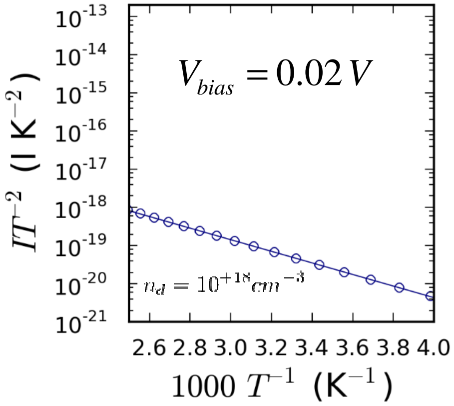
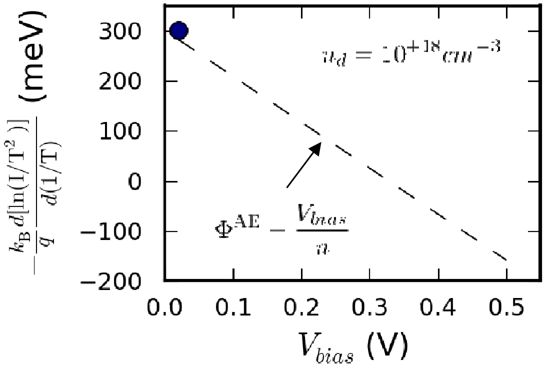




Calculated activation energy curves

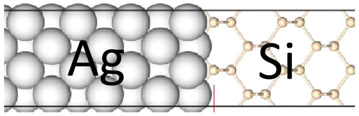
$$I = AA'\,T^{2}e^{-q\Phi_B/k_BT}\left(e^{qV/nk_BT}-1\right) \Rightarrow -\frac{k_B}{q}\frac{d[\ln(I/T^2)]}{d(1/T)} = \Phi^{\mathrm{AE}} - \frac{V_{bias}}{n}$$





Bias dependence

$$\Phi^{\mathrm{AE}} - \frac{V_{bias}}{n}$$



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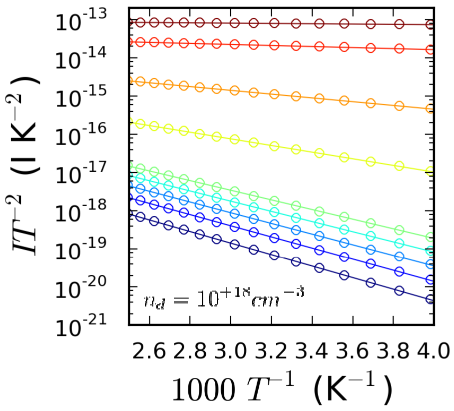
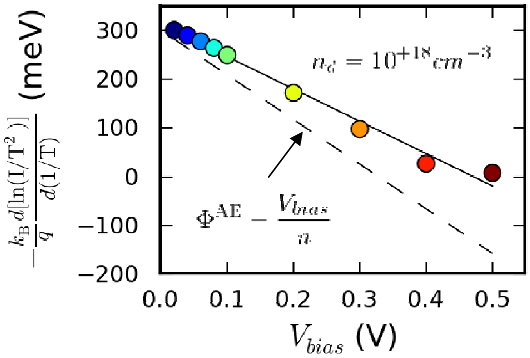
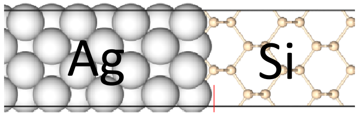




Bias dependence

$$\Phi^{\mathrm{AE}} - \frac{V_{bias}}{n}$$



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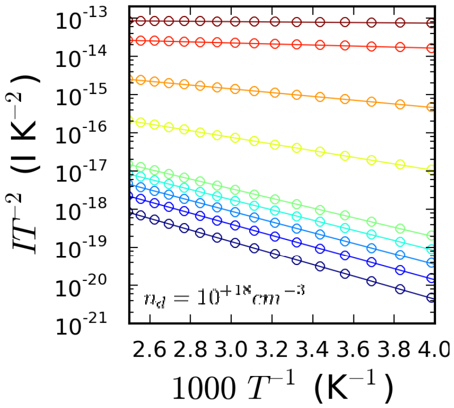
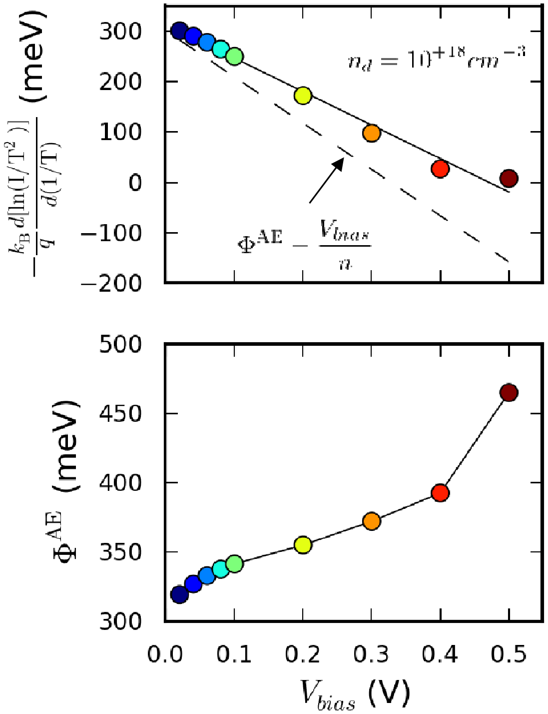


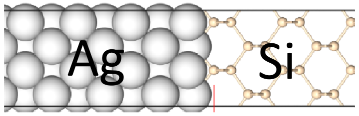


Bias dependence

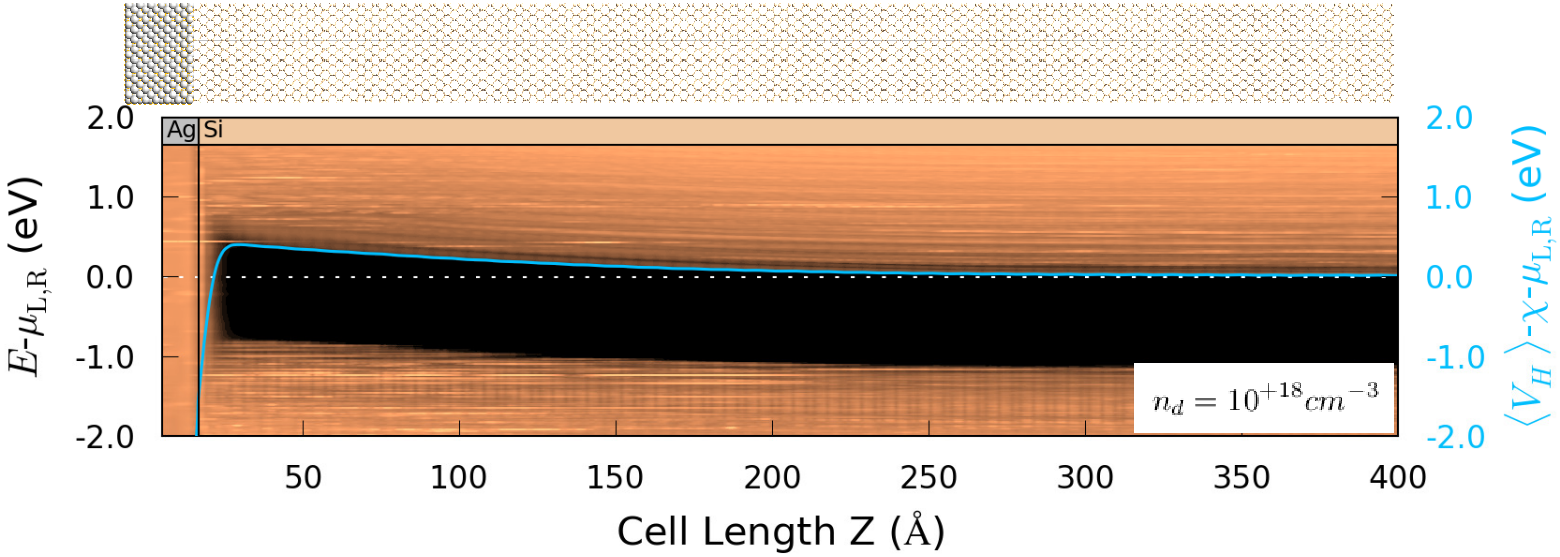
$$\Phi^{\mathrm{AE}} - \frac{V_{bias}}{n}$$

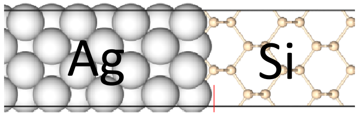
Calculate eff. barrier

$$\Phi^{\mathrm{AE}} = -\frac{k_B}{q}\frac{d[\ln(I/T^2)]}{d(1/T))} + \frac{V_{bias}}{n}$$



Extract the barrier from the electronic structure





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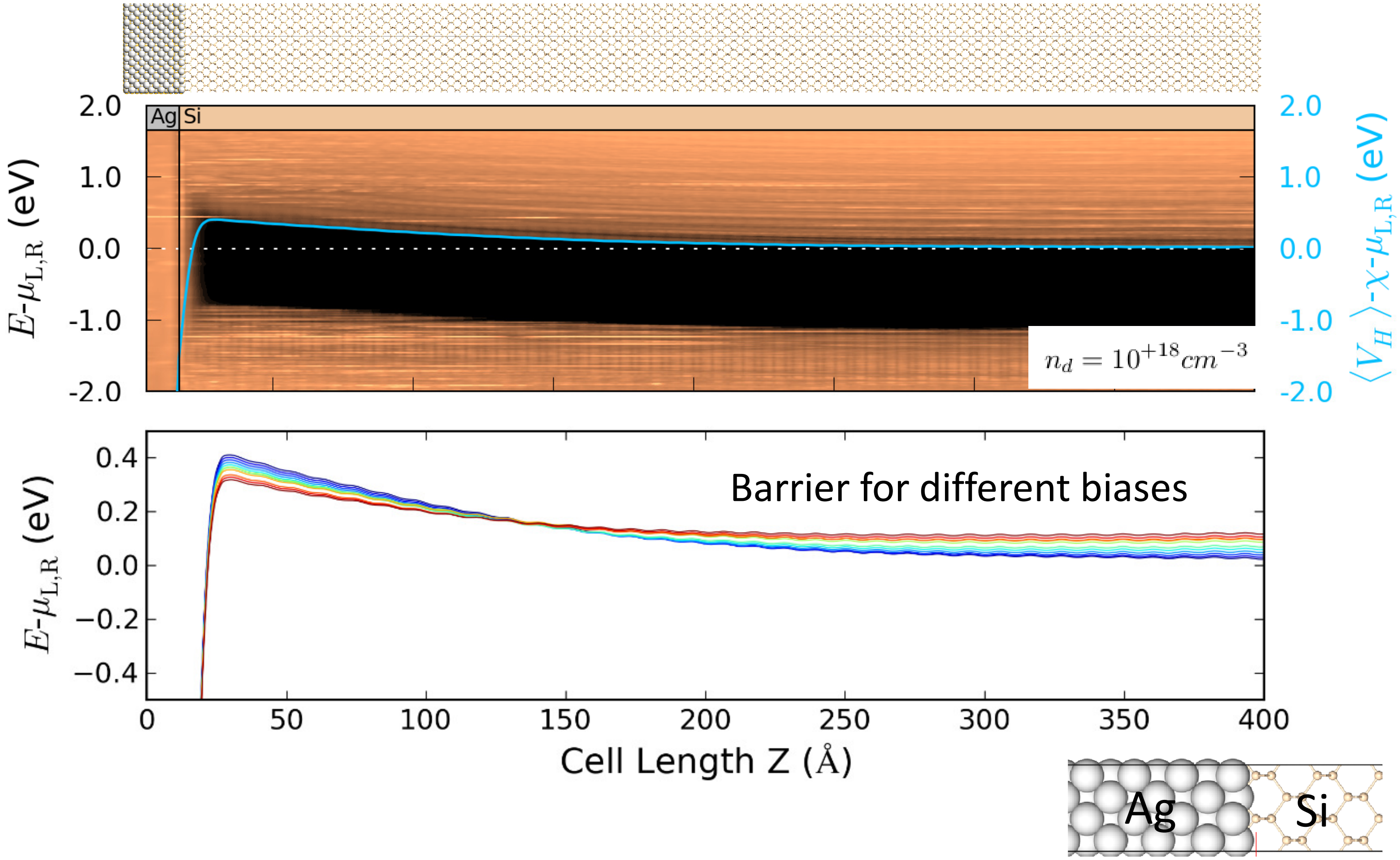
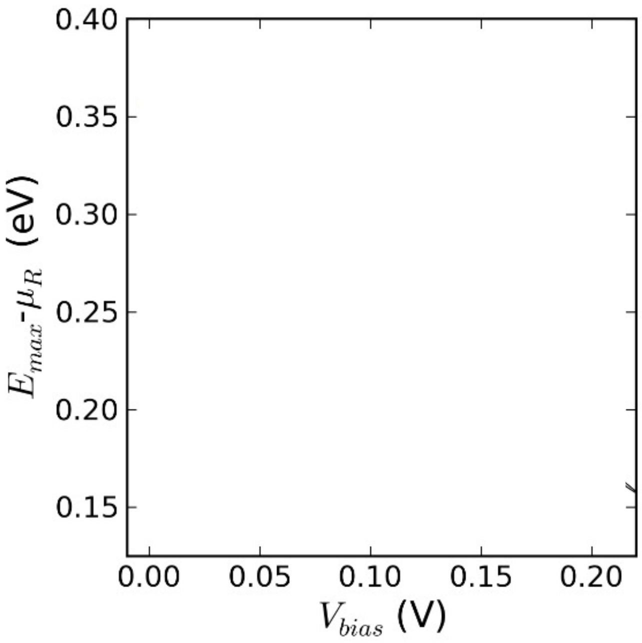
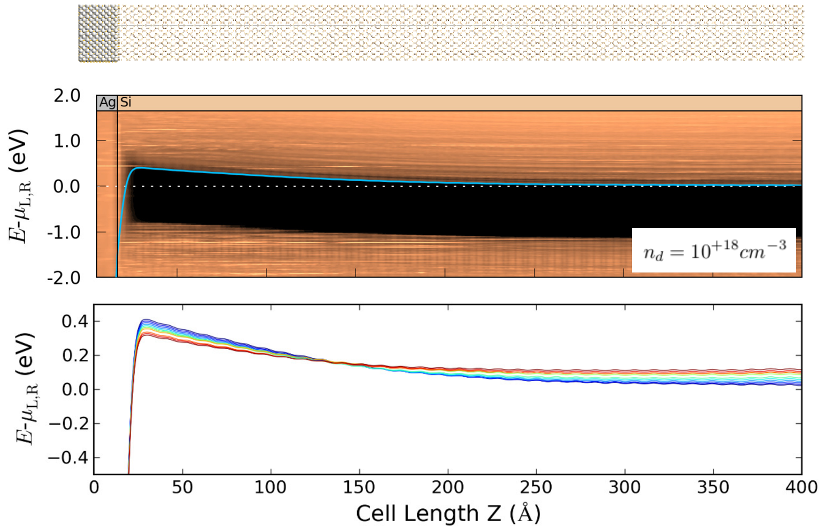
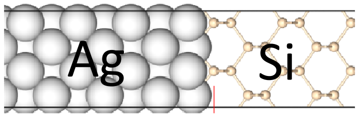


Barrier for different biases

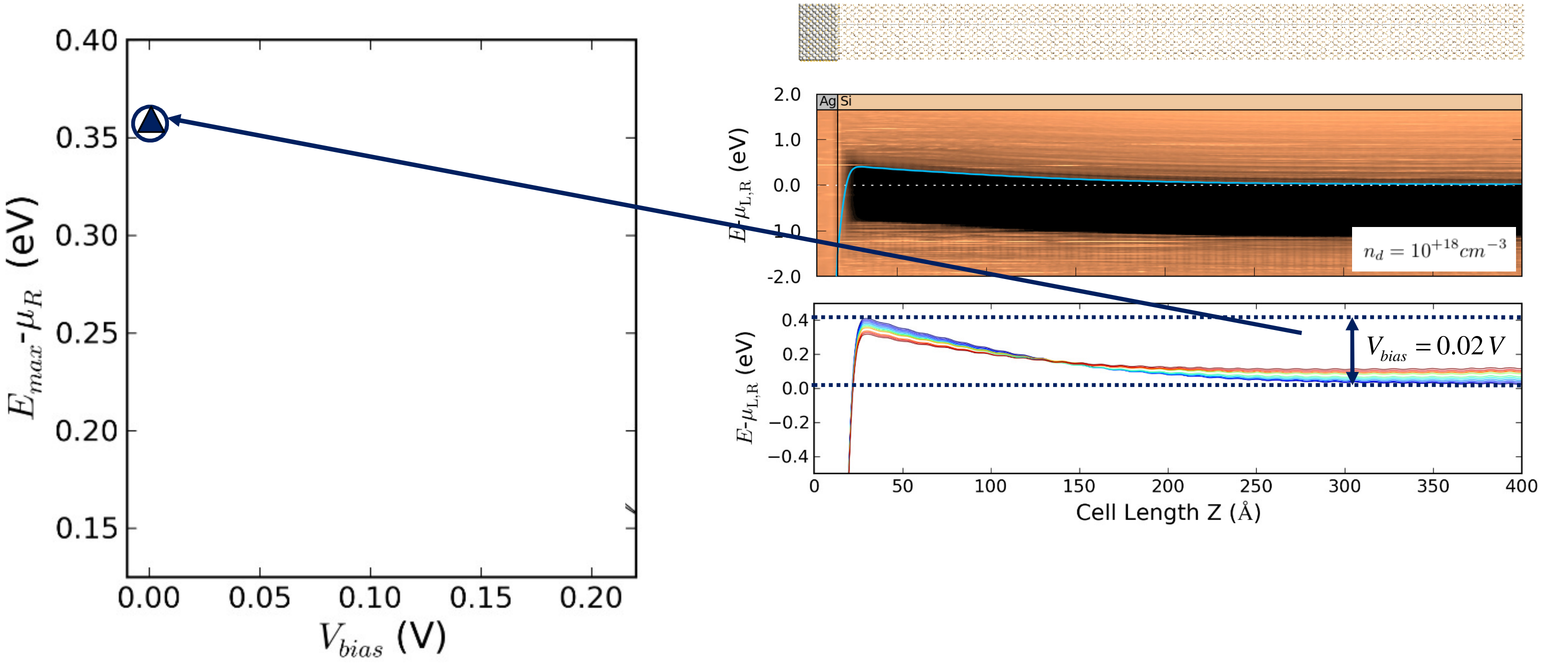
Measure the barrier height

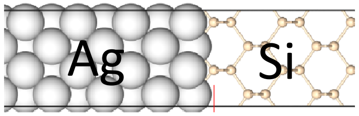




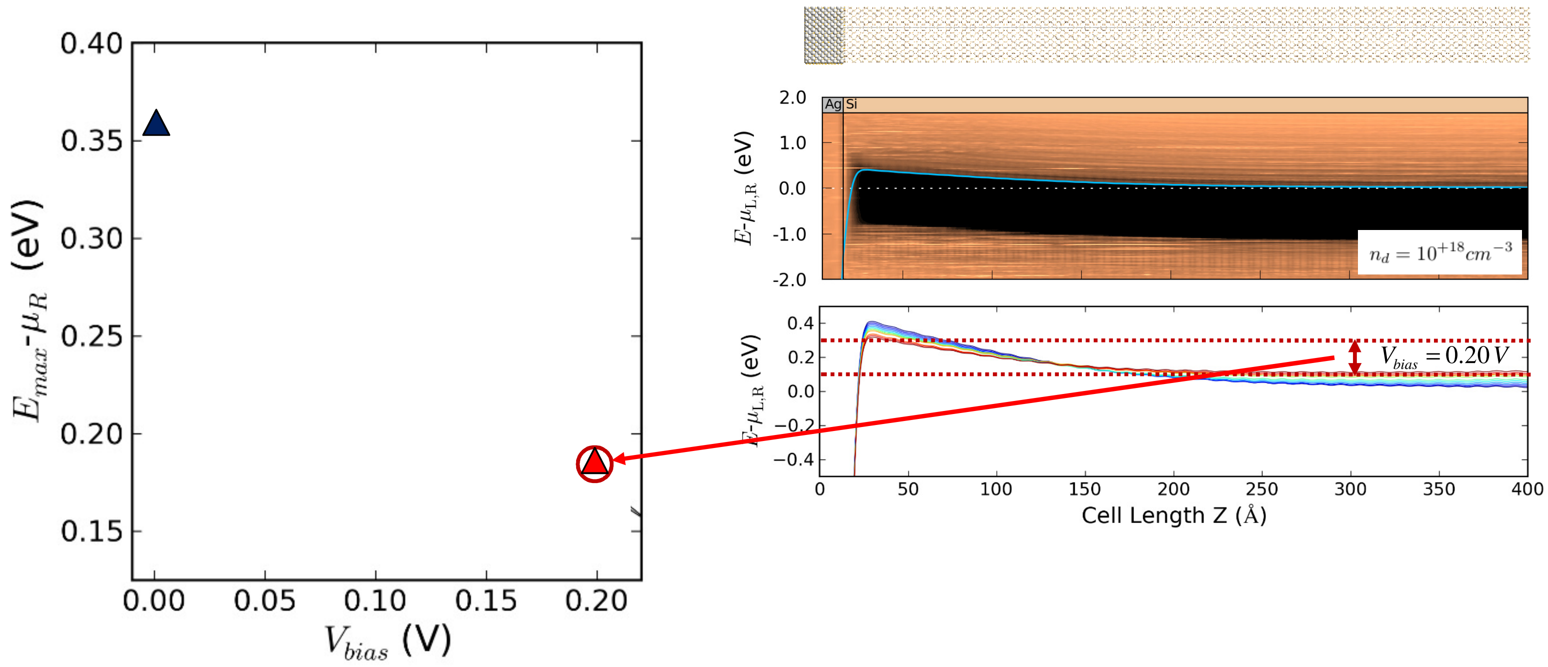


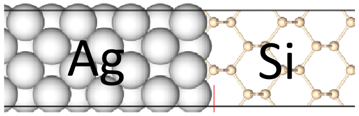
Measure the barrier height



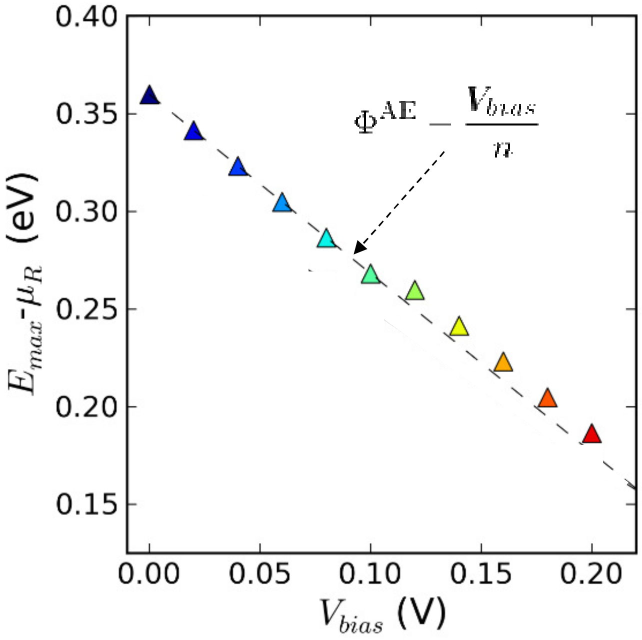


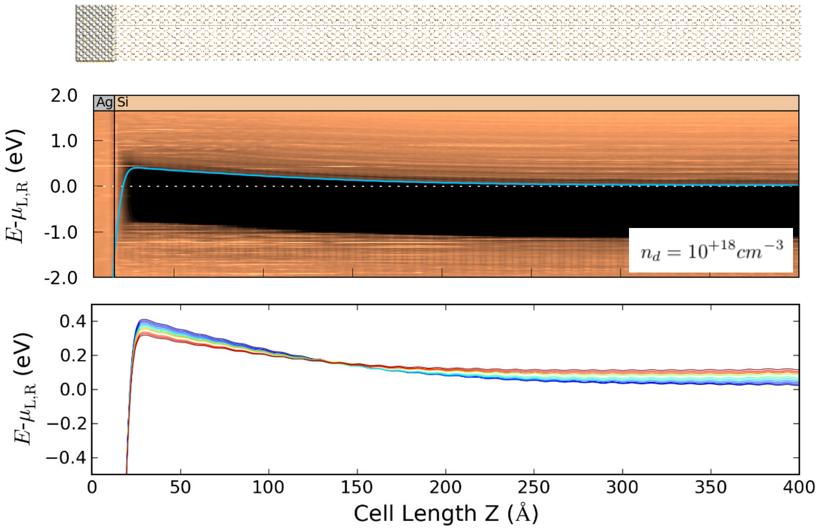
Measure the barrier height

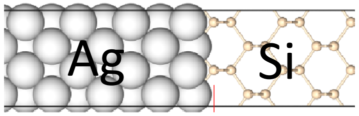




Extract the barrier from the electronic structure







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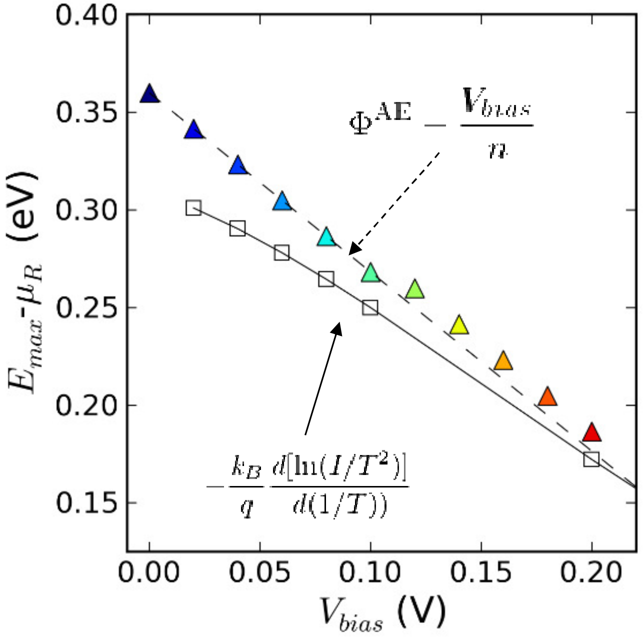
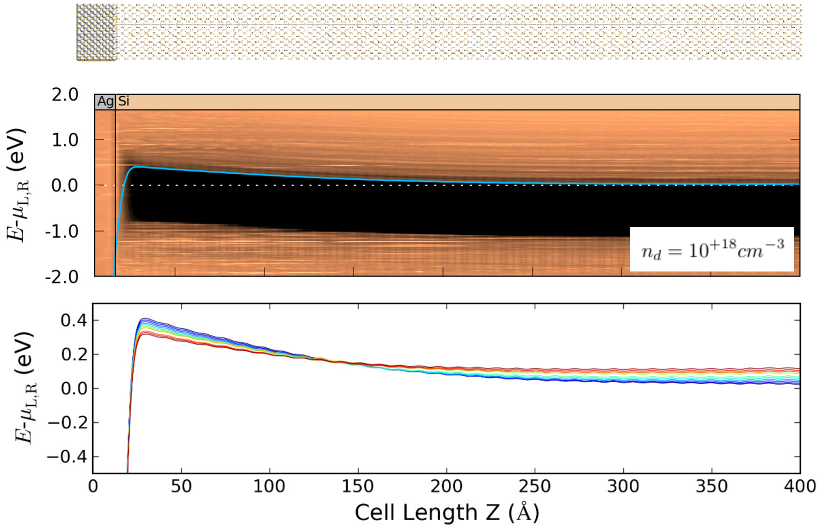
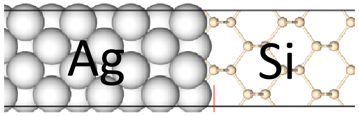
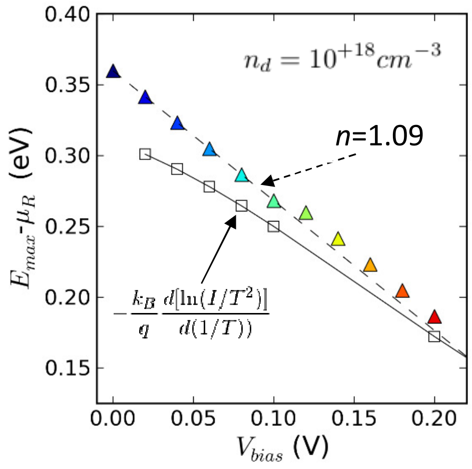
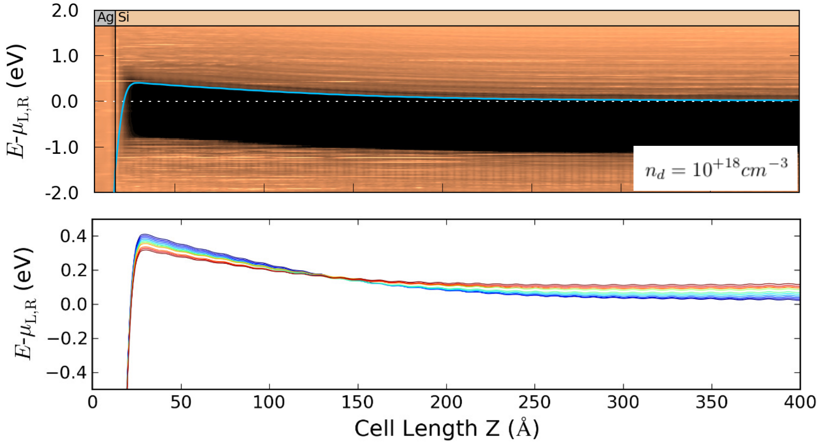


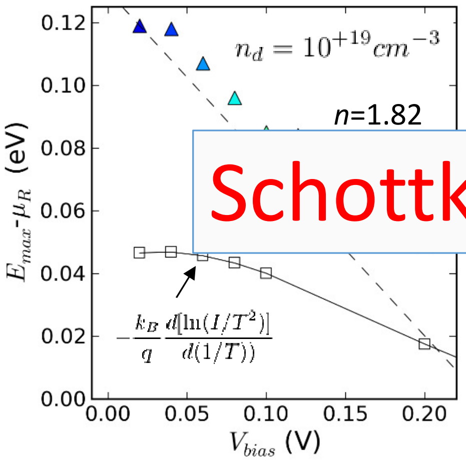


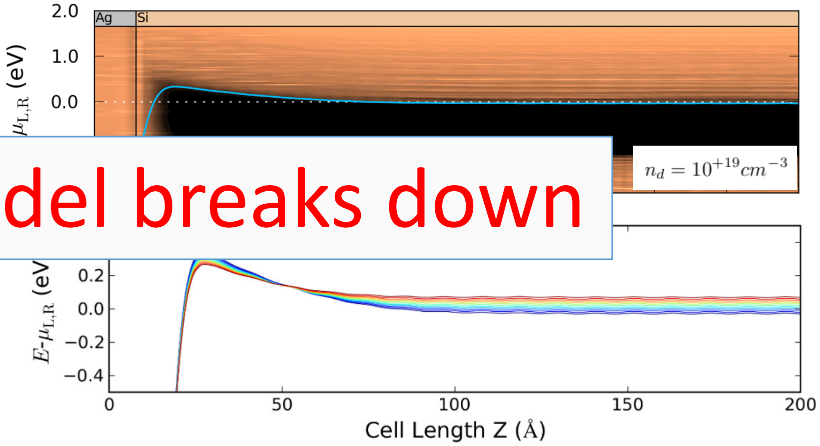


Comparison of different dopings



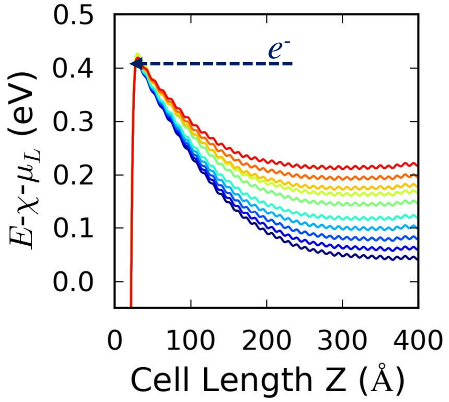


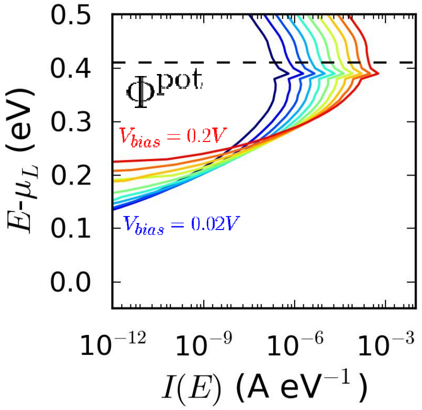




Schottky model breaks down

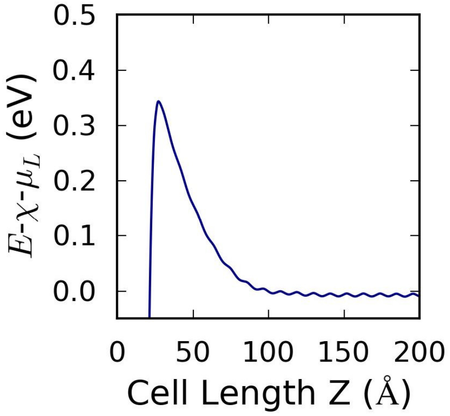
Spectral current analysis: $n_d = 10^{18}$ cm^{-3} vs $n_d = 10^{19}$ cm^{-3}





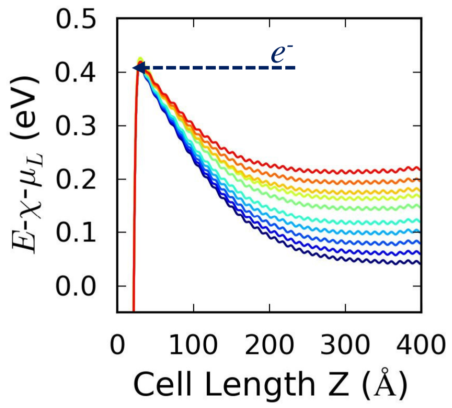
$n_d = 10^{18}$ cm^{-3}

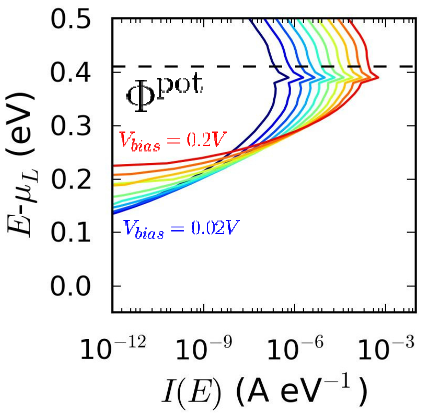
Thermionic emission >> Tunnelling



$n_d = 10^{19}$ cm^{-3}

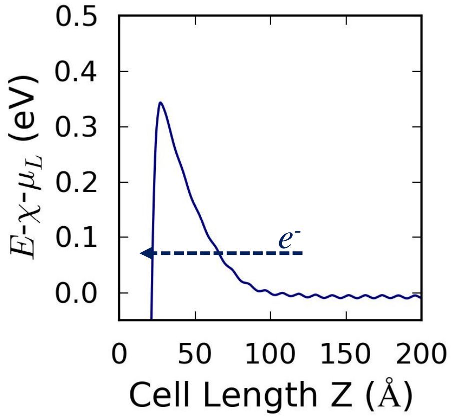
Spectral current analysis: $n_d = 10^{18}$ cm^{-3} vs $n_d = 10^{19}$ cm^{-3}

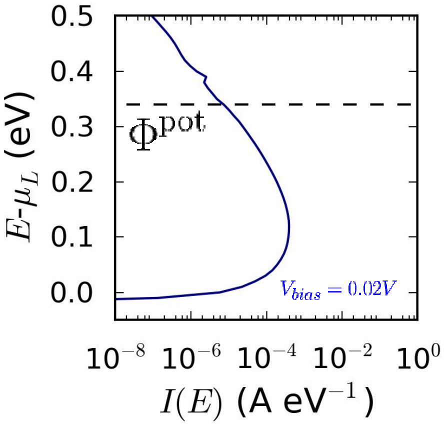




$n_d = 10^{18}$ cm^{-3}

Thermionic emission >> Tunnelling

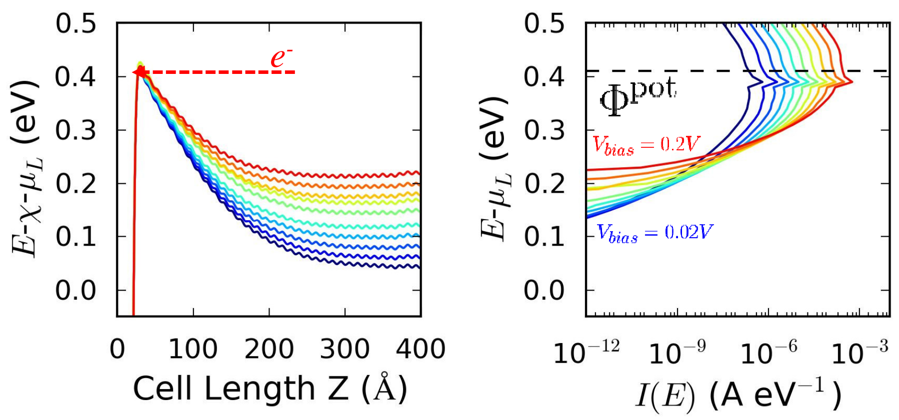




$n_d = 10^{19}$ cm^{-3}

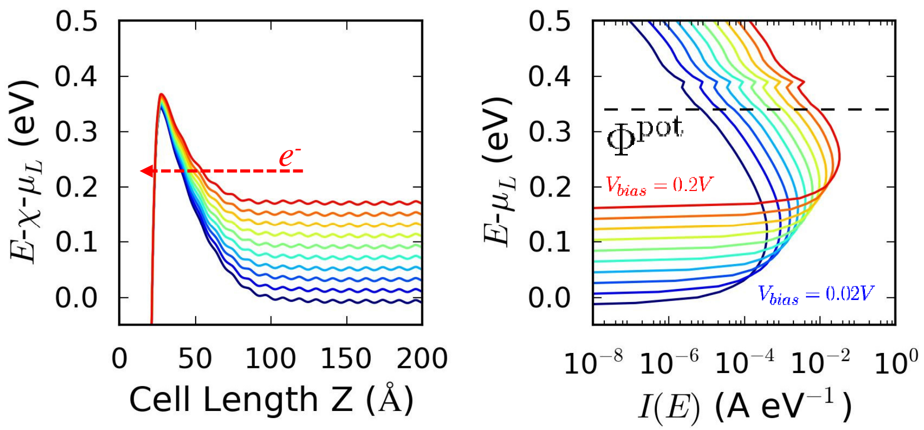
Tunnelling >> Thermionic emission

Spectral current analysis: $n_d = 10^{18}$ cm^{-3} vs $n_d = 10^{19}$ cm^{-3}



$n_d = 10^{18}$ cm^{-3}

Thermionic emission >> Tunnelling



$n_d = 10^{19}$ cm^{-3}

Tunnelling >> Thermionic emission

Outline

QuantumWise

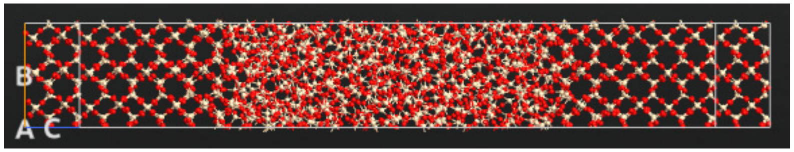
Atomic-scale modelling in the semiconductor industry

Application example: Interfaces

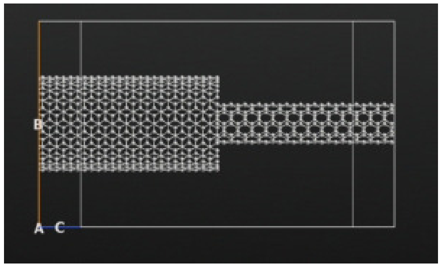
Concluding remarks

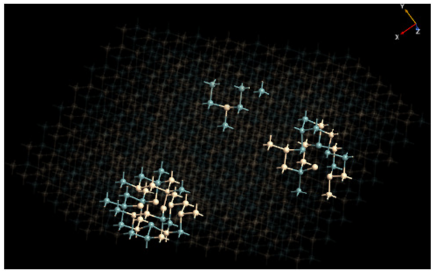
Example applications

- Leakage currents through ultrathin gate oxide layers in MOSFETs
  - Effect of vacancies
- Schottky barrier formation at metal-semiconductor interfaces
  - Fermi level un/pinning due to impurities in the interface
- Contact resistance optimization
- Properties of ultra-thin films
  - M-I-M or M-I-S structures
- Applications in novel memory technologies
  - MRAM, ReRAM, PCRAM, atomic switches
- Systems of reduced dimensionality
  - FinFETs
  - Nanowires (metallic and semiconducting)
  - Nanocrystals



- Tunneling FETs
- Exotic options
  - 2D materials
  - Nanotubes
  - Topological insulators
  - Spintronics
  - Thermionic devices
- Strain engineering
- Grain boundaries
- Piezo/ferroelectric effects
- Thermal resistance of interfaces
- III-V and SiGe
- Vacancy/dopant diffusion





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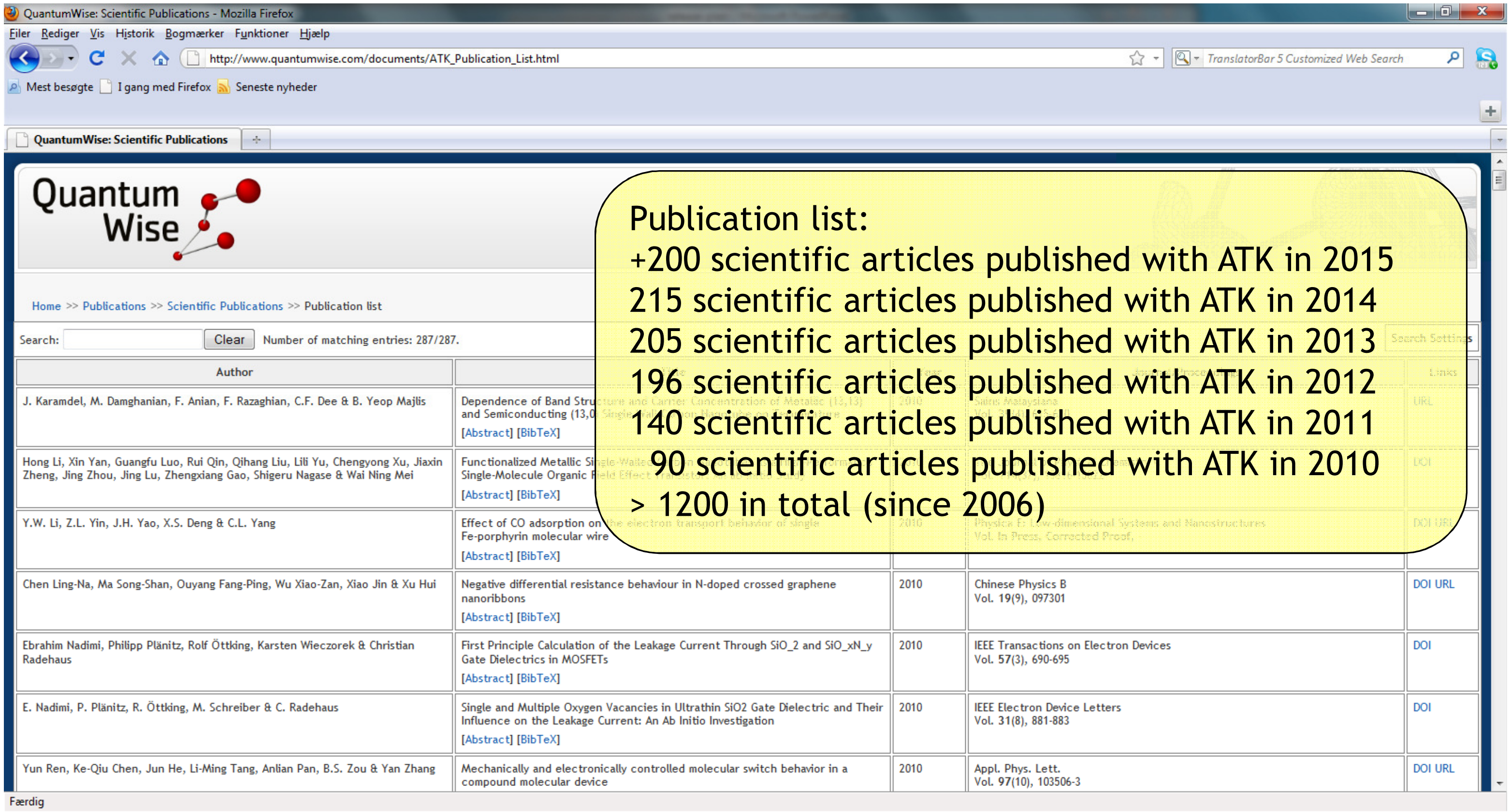

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Hong Li, Xin Yan, Guangfu Luo, Rui Qin, Qihang Liu, Lili Yu, Chengyong Xu, Jiaxin Zheng, Jing Zhou, Jing Lu, Zhengxiang Gao, Shigeru Nagase & Wai Ning Mei	Functionalized Metallic Single-Walled [illegible] Single-Molecule Organic Field Effect Transistor: [illegible] [Abstract] [BibTeX]			DOI
Y.W. Li, Z.L. Yin, J.H. Yao, X.S. Deng & C.L. Yang	Effect of CO adsorption on the electron transport behavior of single Fe-porphyrin molecular wire [Abstract] [BibTeX]	2010	Physica E: Low-dimensional Systems and Nanostructures Vol. In Press, Corrected Proof,	DOI URL
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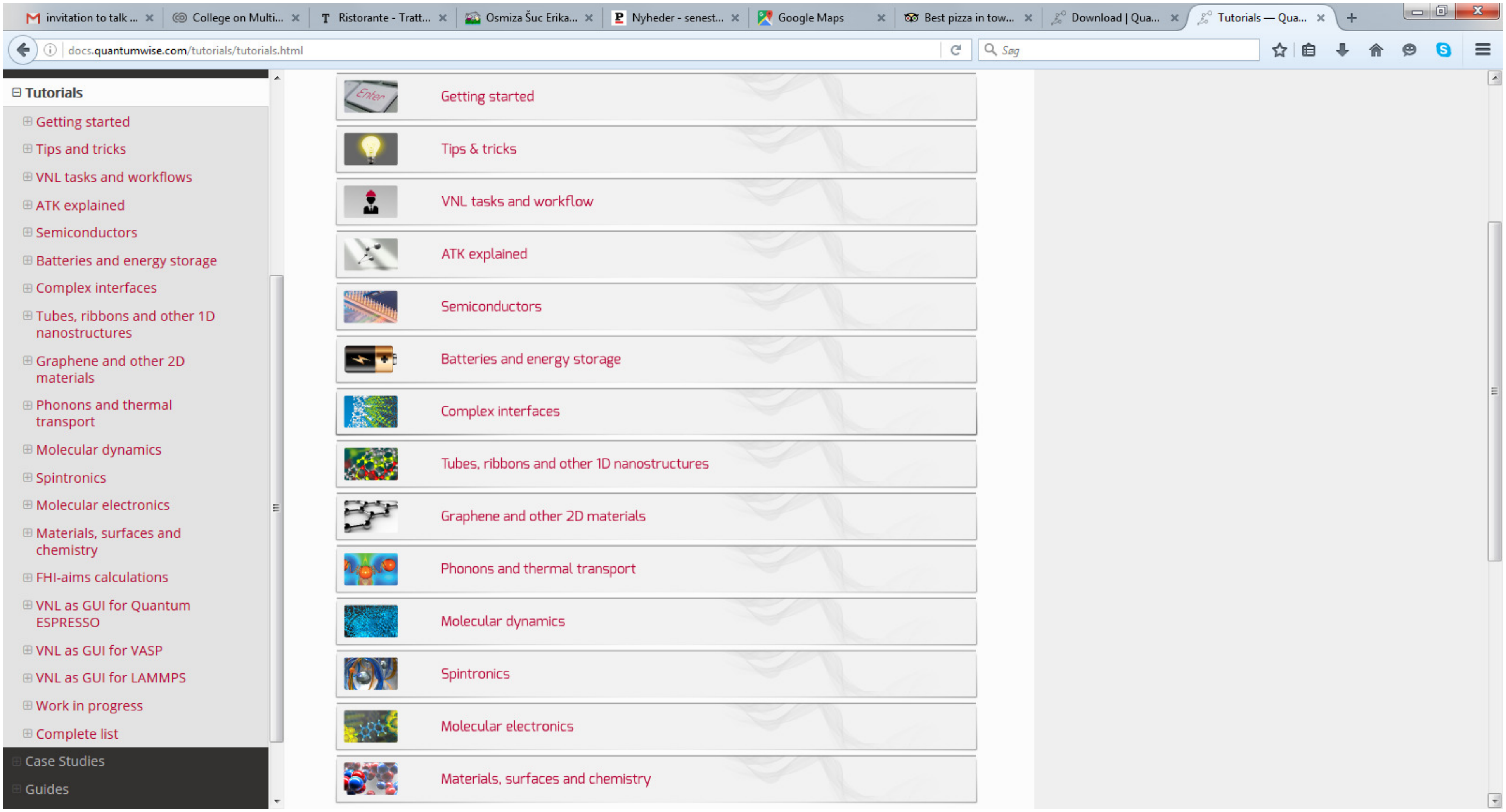

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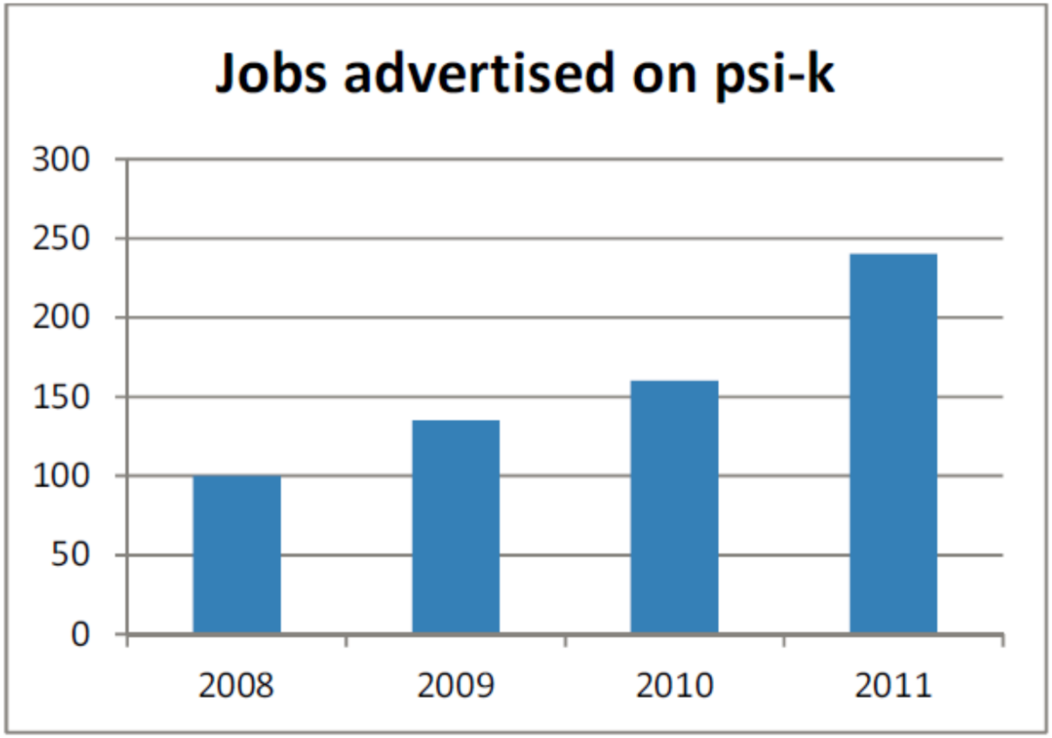
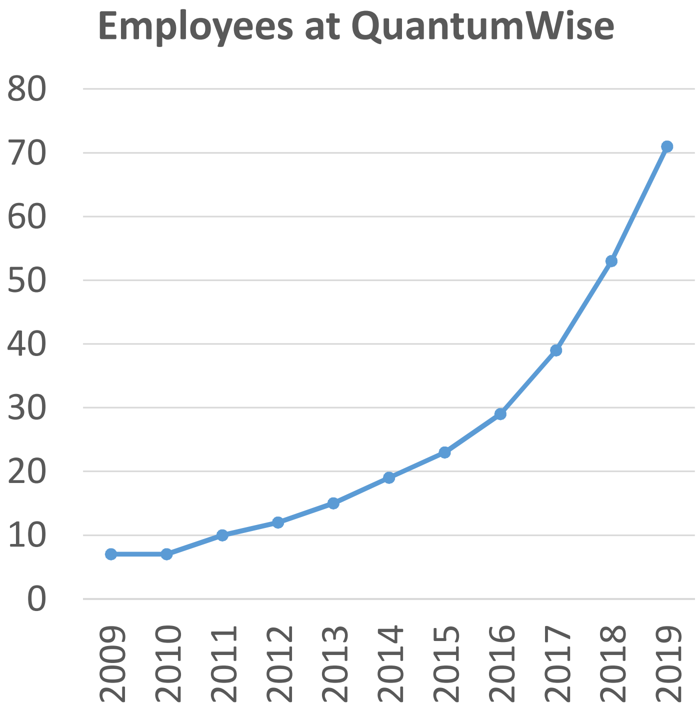
Conclusions from the EMMC

1. Discrete models are well established in the major chemical companies (BASF, Dupont, Dow, Sumitomo Chemical) since several decades. The expansion to smaller chemical companies is slow.
2. The use of e/a/m modelling in industries dealing with solid state materials is emerging
3. The key bottlenecks are
    - Shortcomings in the intrinsic capabilities
    - Lack of industry-ready integrated, standardized, interoperable software solutions
    - Lack of trained translators
    - Coupling between the atomistic and the continuum scales
4. Government investments are often guided by academic objectives, not progressing the transfer of modelling software to industrial endusers
5. Continuum modelling is well established with a few large commercial software owners. Discrete models is less established with many scattered small commercial and academic software owners.
6. Strong academic community in Europe within discrete models.

High demand for experts in electronic-structure theory





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