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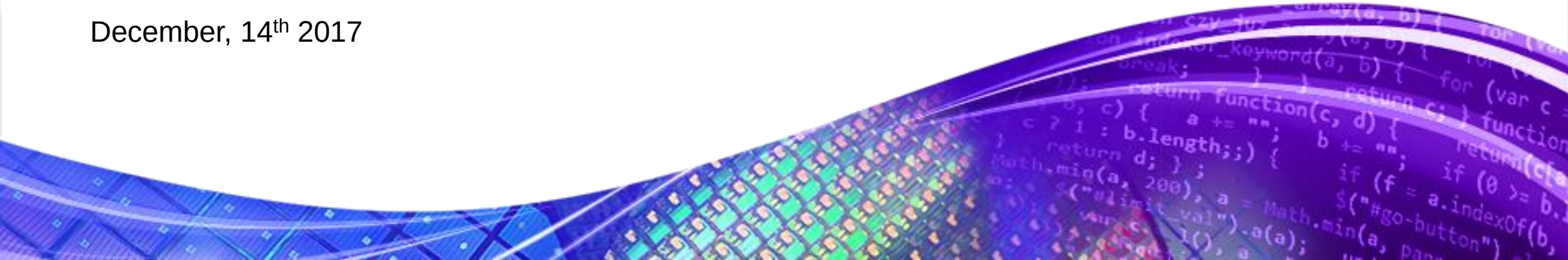
Silicon to Software™

How to include electron-phonon scattering effects in large-scale atomistic simulations

Daniele Stradi
Ulrik Grønbjerg Vej-Hansen

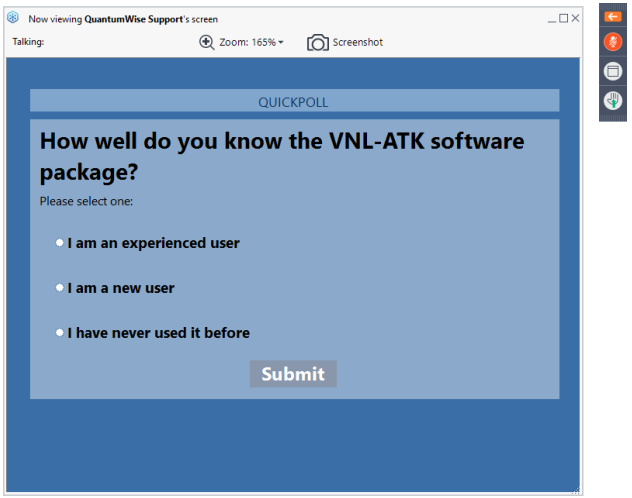
Synopsys QuantumWise

December, 14th 2017

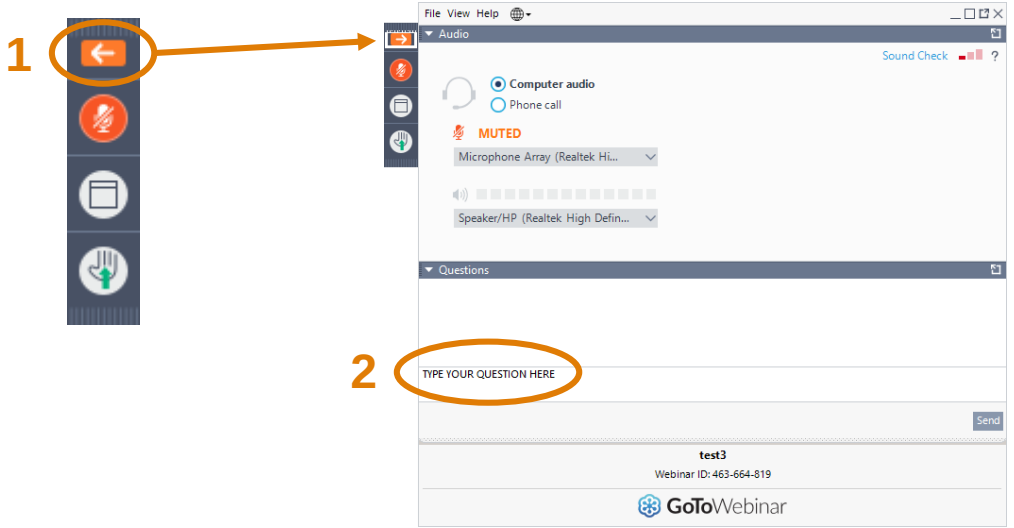


General info about this seminar.

- Two **polls** will be distributed during the webinar. The window will change temporarily to allow the attendees to answer the poll. The duration of each poll will be of 30 seconds.



- You can **ask questions** by clicking on the **orange button** (1). A new window will open in which you can type your question (2). As many questions as possible will be addressed by the presenters in the Q&A session at the end of the webinar.



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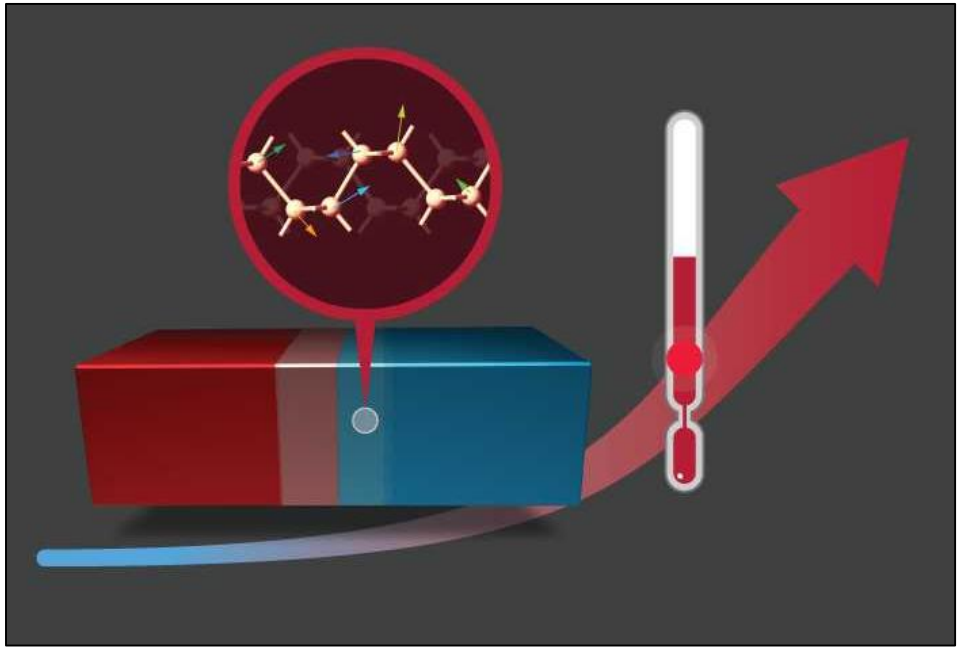
Outline.

- **Overview of the STD – Landauer (Special Temperature Displacement – Landauer) method in ATK.**
- **Introduction to e-ph scattering effects.**
- **Role of e-ph scattering effects in the performance of electronic devices.**
- **Atomistic simulations of ultra-scaled electronic devices using ATK.**
- **The STD-Landauer method.**
  - Target applications.
  - Theory.
  - General considerations.
- **How to setup, run and analyze an STD-Landauer calculation in ATK.**

Overview of the STD – Landauer (Special Temperature Displacement – Landauer) method in ATK.

- **Parameter-free first-principles electronic transport simulations** of devices can be performed in **ATK** using density functional theory (**DFT**) combined with Non-equilibrium Green's function (**NEGF**). See:
  - *https://docs.quantumwise.com/manuals/ATKDFT.html*
  - *https://docs.quantumwise.com/manuals/NEGF.html*
- **STD-Landauer** is a computationally efficient method to include electron-phonon scattering effects in **ATK** electronic transport simulations using DFT-NEGF.
- It makes it possible to calculate finite-temperature characteristics of devices using only few computationally intensive **ATK** device simulations.
- It is targeted at technologically relevant and structurally homogeneous systems.



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Introduction to e-ph scattering effects.

The total Hamiltonian of the system can be formally separated in three terms: $\hat{H}_{\mathrm{tot}} = \hat{H}_{\mathrm{e}} + \hat{H}_{\mathrm{ph}} + \hat{H}_{\mathrm{e-ph}}$

Electrons

Phonons

Interaction between electrons and phonons

Cardona, Yu *Fundamentals of Semiconductors* (Springer, 2005)

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Electrons | **Phonons** | **Interaction between electrons and phonons**

- Within the **Born-Oppenheimer approximation**:
  - The electronic Hamiltonian depends parametrically on the nuclear coordinates;
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$$\hat{H}_{\mathrm{e}} = \hat{H}_{\mathrm{e}}^{0} + \sum_{i,j} \left.\frac{\partial \hat{H}_e}{\partial Q_{ij}}\right|_{\mathbf{Q}=0} Q_{ij} + \cancel{\ldots}$$

We neglect higher-order terms

Electron-phonon interaction

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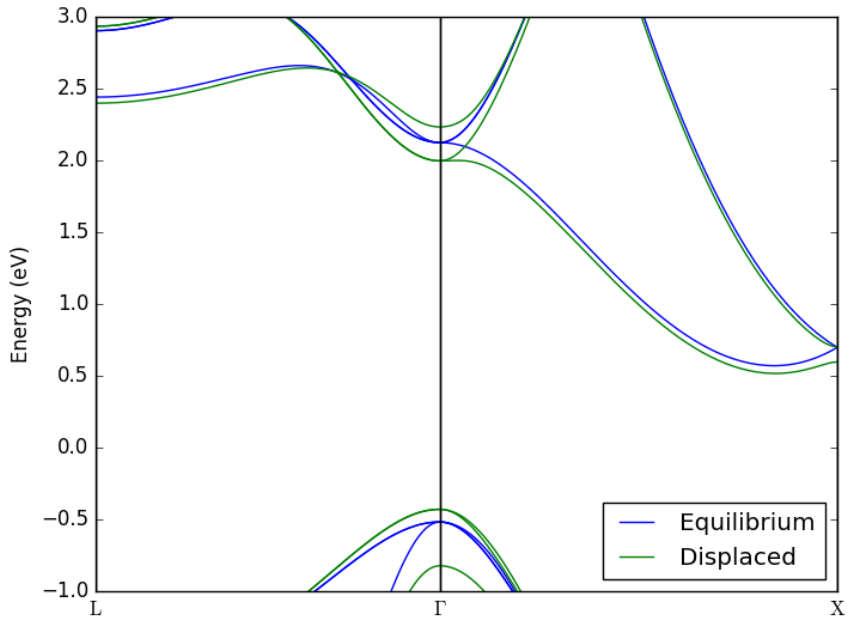
We neglect higher-order terms

Electron-phonon interaction

- Assuming that the energy dispersion of a band is known, the e-ph interaction can be understood as a **shift of the electronic band energy caused by a static displacement** of the atoms:

$$\left.\frac{\partial \hat{H}_e}{\partial Q_{ij}}\right|_{\mathbf{Q}=0} Q_{ij} \approx \left.\frac{\partial \hat{E}_{n\mathbf{k}}}{\partial Q_{ij}}\right|_{\mathbf{Q}=0} Q_{ij}$$

Band structure of Silicon using equilibrium and distorted structures



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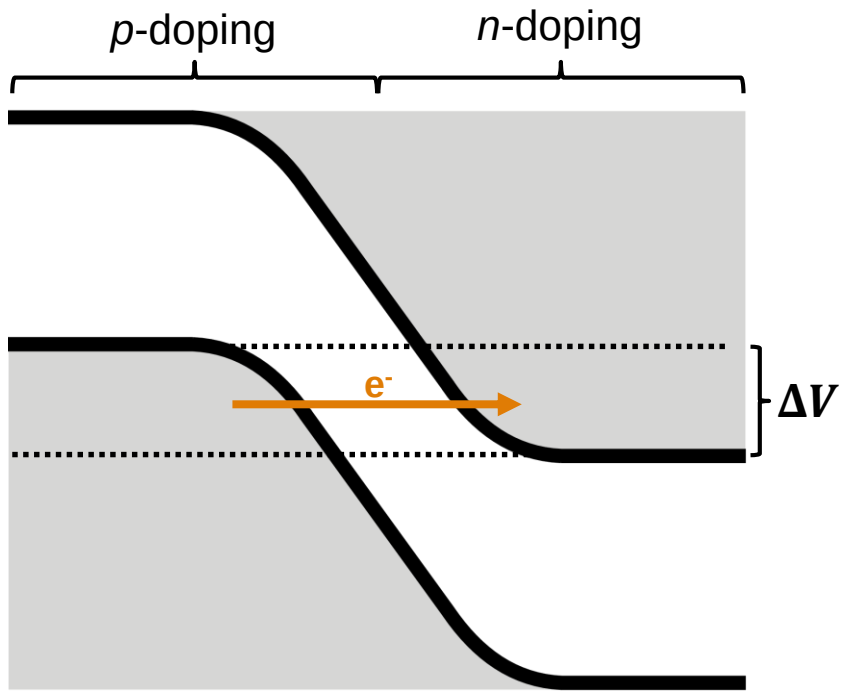
Role of e-ph scattering effects on the performance of electronic devices.

- As transistors scale below 10 nm, **quantum mechanical (QM) phenomena** start playing an important role in the performance of the transistors.
- **Direct QM tunneling** between the source and drain electrodes can become important due to scaling down of channel length.
- **The tunneling current can be affected by electron-phonon scattering effects**, ultimately modifying the characteristics of the transistor.



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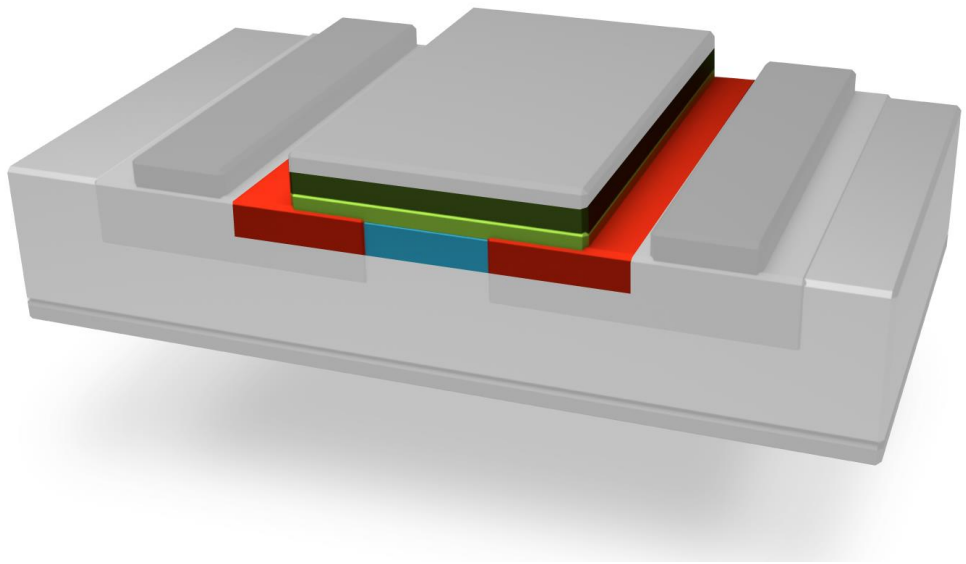
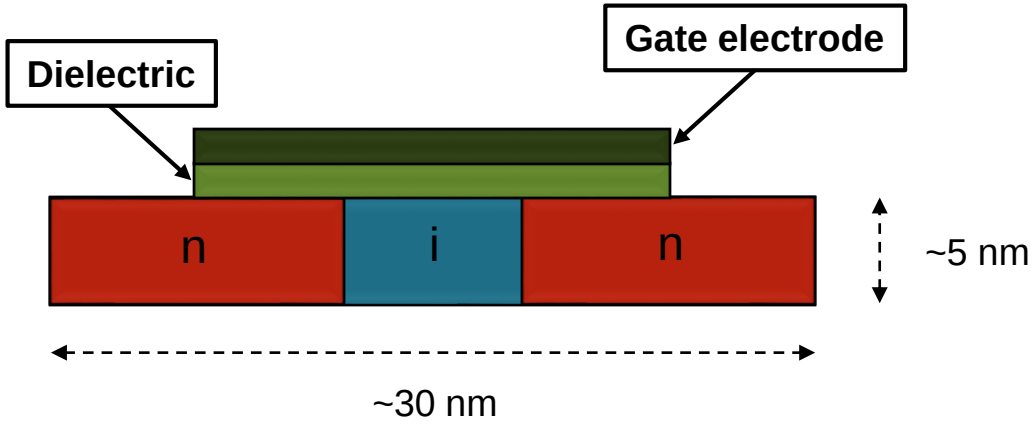
Atomistic simulations of ultra-scaled electronic devices.





- Atomistic simulations using **ATK** and *ab-initio* density functional theory (DFT) can nowadays be used to simulate **systems of ~1000 atoms**, which allows one to investigate **small but realistic models of the transistor**.
- These model systems are still considered as **large-scale in *ab-initio* theory**.
- **Conventional perturbative approaches used to include e-ph effects** are **too computationally demanding** to be used routinely in combination with these large-scale models.

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The STD-Landauer method: Introduction and target applications.

- **STD:** a Special Thermal Displacement is used to account for the effect of temperature on the atomic lattice.
- **Landauer:** Landauer theory is used to calculate the current between the source and drain electrodes.

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- **STD:** a Special Thermal Displacement is used to account for the effect of temperature on the atomic lattice.
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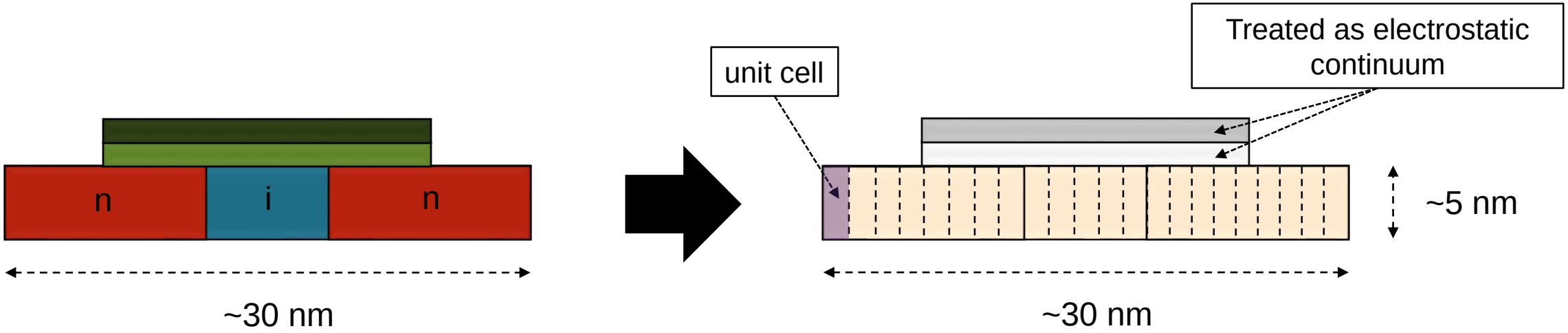
- The STD-Landauer method is designed to include electron-phonon scattering effects in **large-scale homogeneous devices formed by a large number of repetitions of a single unit cell** along the transport direction.



- Example of applications: *p-n* junctions, *n-i-n* junctions.

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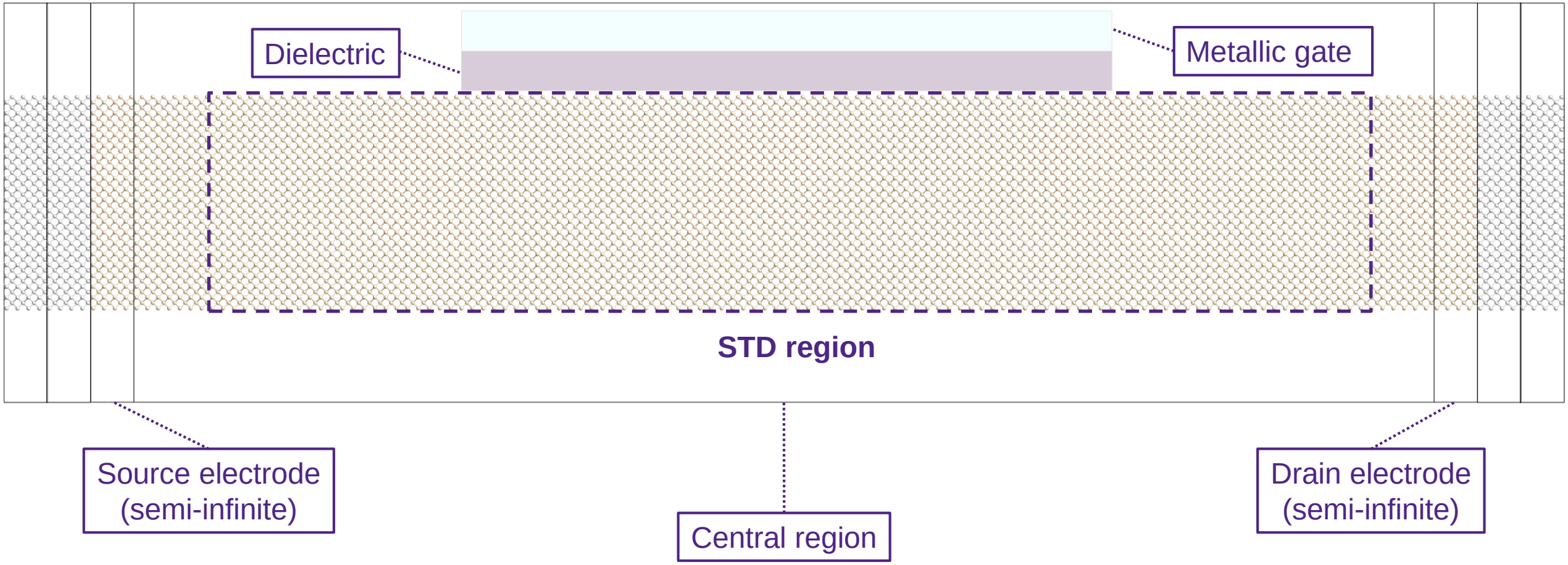
The STD-Landauer method: Introduction and target applications.

- A practical example of an system suited for an STD-Landauer calculation with **ATK**:



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The STD-Landauer method: Theory.

- Williams-Lax theory for optical adsorption [*Phys. Rev. Lett.* **115**, 177401 (2015) and references therein]:

$$\underbrace{\langle \epsilon_2(\omega, T) \rangle}_{\text{Expectation value at temperature T}} = Z^{-1} \sum_n \exp(-E_n/k_B T) \underbrace{\langle \epsilon_2(\omega, \{\mathbf{u}_\lambda\}) \rangle_n}_{\text{Expectation value of state } n \text{ with nuclear displacements } \{\mathbf{u}_\lambda\}}$$

  - The **expectation value** of the imaginary part of the dielectric constant ϵ_2 at temperature T is given by a **canonical average** over all the expectation values of ϵ_2 for all possible nuclear displacements $\{\mathbf{u}_\lambda\}$.

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How to perform efficiently the configurational sampling over all the possible nuclear displacements $\{\mathbf{u}_\lambda\}$?

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The STD-Landauer method: Theory.

Special displacement to approximate the correct thermally-averaged observable, $\langle \mathcal{T}(E,T) \rangle \approx \mathcal{T}_{STD}(E,\{\mathbf{u}_\lambda\})$.

- **1st step:** solution of $\langle \mathcal{T}(E,T) \rangle$ around the equilibrium configuration:

2. Evaluate integral analytically

$$\langle \mathcal{T}(E,T) \rangle = \prod_\lambda \int du_\lambda \frac{\exp(-u_\lambda^2/2\sigma_\lambda^2)}{\sqrt{2\pi}\sigma_\lambda} \mathcal{T}(E,\{\mathbf{u}_\lambda\})$$

1. Expand in a Taylor series

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1. Expand in a Taylor series

0th order | 2nd order | 4th order and higher

  - Only **even order terms** are present.
  - The width σ is related to the **mean square displacement** $\langle \mathbf{u}_\lambda^2 \rangle = \sigma_\lambda^2(T)$, therefore $\mathbf{u}_\lambda = s_\lambda \sigma_\lambda\,(T)$.
  - Assuming that all the phonons have the same contribution, $s_\lambda = \pm 1$. **The sign for each phonon λ is undefined.**

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The STD-Landauer method: Theory.

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- **2nd step:** solution of $\mathcal{T}_{STD}(E,\{\mathbf{u}_\lambda\})$ around the equilibrium configuration and choice of the appropriate signs s_λ:

0th order | 1st order | 2nd order | 3rd order and higher

$$\mathcal{T}_{STD}(E,\{\mathbf{u}_\lambda\}) = \mathcal{T}_0(E) + \sum_\lambda s_\lambda \frac{\partial \mathcal{T}(E,\{\mathbf{u}_\lambda\})}{\partial \mathbf{u}_\lambda}\sigma_\lambda + \sum_{\lambda\lambda'} s_\lambda s_{\lambda'} \frac{\partial^2 \mathcal{T}(E,\{\mathbf{u}_\lambda\})}{\partial \mathbf{u}_\lambda \mathbf{u}_{\lambda'}}\sigma_\lambda \sigma_{\lambda'} + \mathcal{O}(\sigma^3)$$

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- The relation $\langle \mathcal{T}(E,T) \rangle \approx \mathcal{T}_{STD}(E,\{\mathbf{u}_\lambda\})$ is verified when:
  - The signs s_λ are chosen so that $S = (s_1, s_2, s_3, s_4, \dots) = (+,-,+,-,\dots)$.
  - The number of phonons $N_\lambda \to \infty$ and successive phonon modes are nearly degenerate $(\omega_\lambda \approx \omega_{\lambda+1})$.

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$0\ if\ \lambda \neq \lambda'$

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  - The signs s_λ are chosen so that $S = (s_1, s_2, s_3, s_4, \dots) = (+,-,+,-,\dots)$
  - The number of phonons $N_\lambda \to \infty$ and successive phonon modes are nearly degenerate $(\omega_\lambda \approx \omega_{\lambda+1})$
- For **large systems with a high repetitions of unit cells** along the transport direction, these conditions are met using the **special displacements**:

$$\mathbf{u}_{STD} = \sum_\lambda (-1)^{\lambda-1} \sigma_\lambda \mathbf{e}_\lambda$$

- Normal mode of phonon λ at $T = 0K$
- Can be calculated using ATK

T-dependent width

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The STD-Landauer method: General considerations.

- The STD-Landauer method uses a **single special displacement** to provide a **temperature-dependent transmission $\mathcal{T}_{STD}(E,\{u_\lambda\})$ that approximates the correct thermally-averaged observable $\langle\mathcal{T}(E,T)\rangle$;**
- The method **applies to systems with a high degree of repetition of the same basic unit cell** along the transport direction since it relies on cancellations of errors between degenerate phonon modes;
- The method is **best suited for systems with bulk-like nonlocalized vibrations;**
- Computationally efficient force fields [Modelling Simul. Mater. Sci. Eng. 25 085007 (2017)] are available in **ATK** to calculate the phonons of a large selection of technologically important systems. Therefore:
  1. The phonons can be evaluated at essentially zero computational cost.
  2. Only $\mathcal{T}_{STD}(E,\{u_\lambda\})$ is evaluated using density functional theory (DFT).

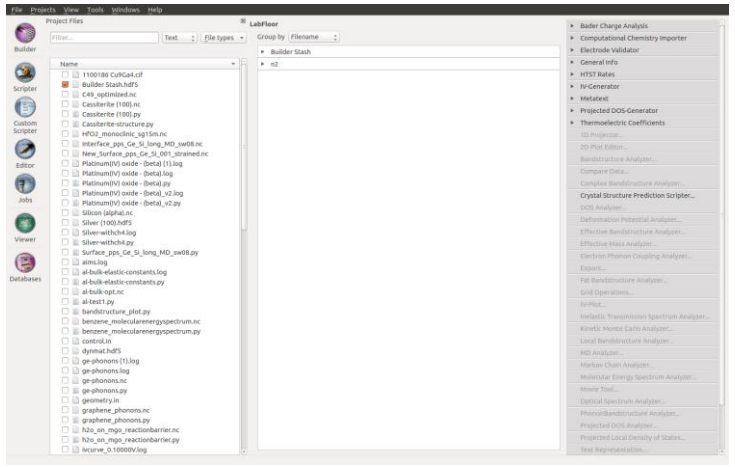
Only one computationally intensive DFT calculation is needed to evaluate $\mathcal{T}_{STD}(E,\{u_\lambda\})$ at a given temperature.

How to setup, run and analyze an STD-Landauer calculation in VNL and ATK.

- Using the Standard Thermal Displacement in ATK and VNL
- Live demonstration in VNL
- IV curve in silicon pn-junction with and without electron-phonon scattering effects
- Current in a silicon n-i-n double-gated MOSFET

Using the Standard Thermal Displacement in ATK/VNL

What is needed to use the STD method in ATK/VNL?



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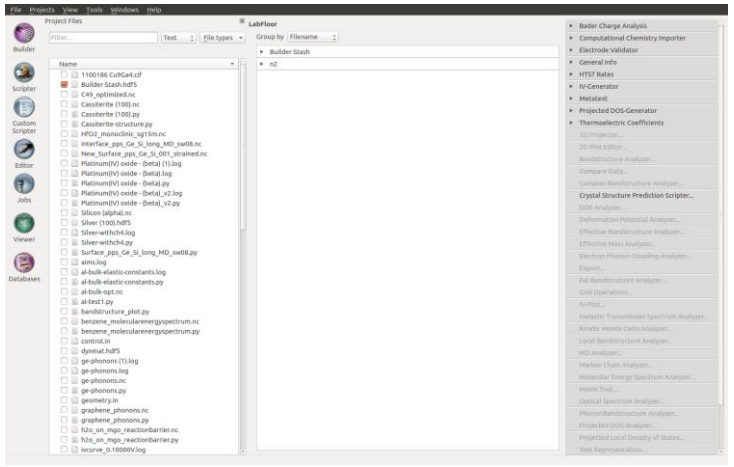
Using the Standard Thermal Displacement in ATK/VNL

What is needed to use the STD method in ATK/VNL?

- ❑A configuration of atoms, such as a Silicon pn-junction



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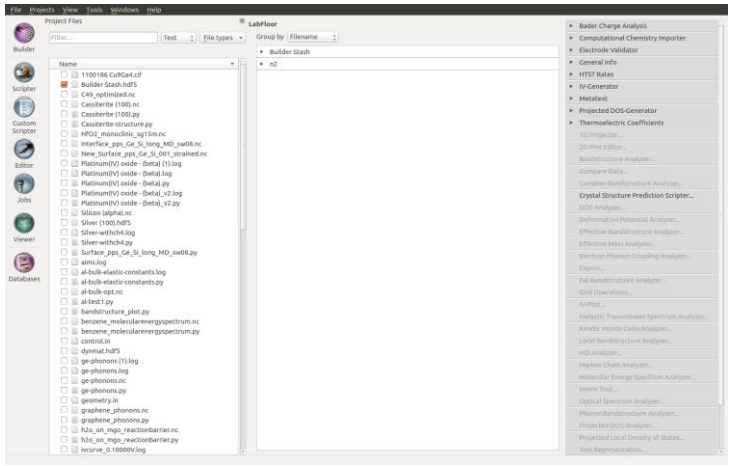
Using the Standard Thermal Displacement in ATK/VNL

What is needed to use the STD method in ATK/VNL?

- ❑A configuration of atoms, such as a Silicon pn-junction
- ❑A dynamical matrix, containing information on the phonon modes



D_{ij}

dyn-mat-demo.hdf5
DynamicalMatrix_0

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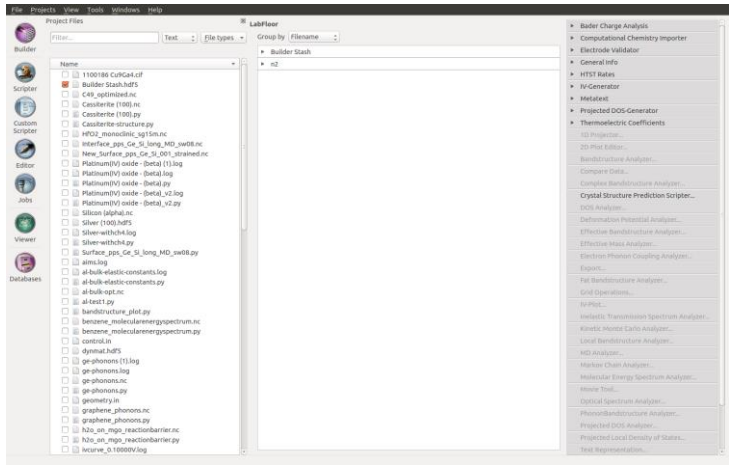
Using the Standard Thermal Displacement in ATK/VNL

What is needed to use the STD method in ATK/VNL?

- ❑A configuration of atoms, such as a Silicon pn-junction
- ❑A dynamical matrix, containing information on the phonon modes
- ❑A user-defined temperature



D_{ij}

dyn-mat-demo.hdf5
DynamicalMatrix_0

$T = 300K$

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Live demonstration with VNL

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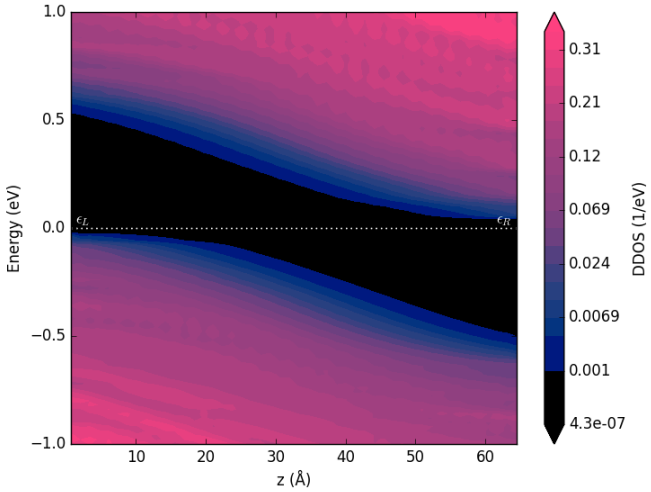
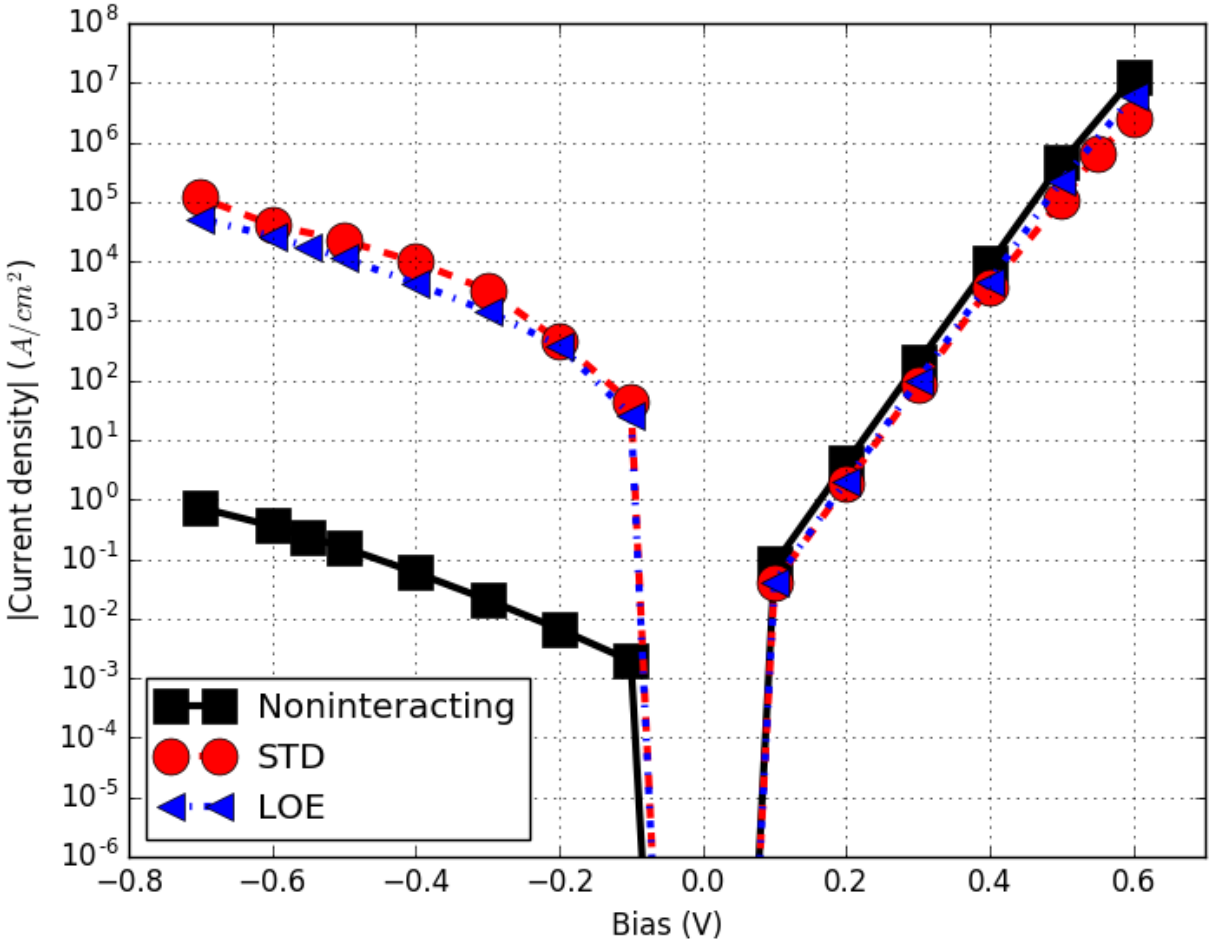
IV Curve for silicon pn-junction at 300 K – using STD

- Current under reverse bias is strongly influenced by electron-phonon scattering effects
- Agreement between the more advanced methods (LOE) and the Special Thermal Displacement (STD) method for the current





https://docs.quantumwise.com/casestudies/std_transport/std_transport.html

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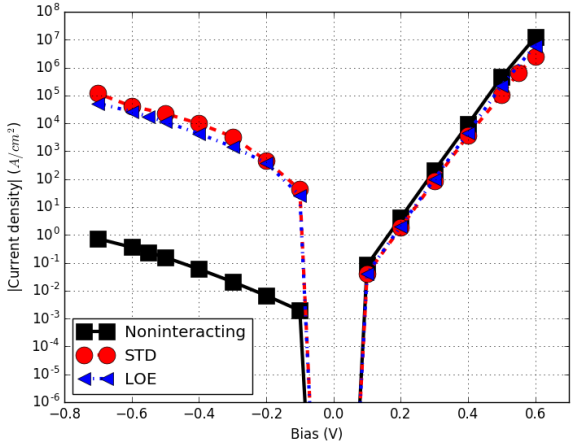
Comparing the numbers



I_{ON}/I_{OFF} :

Bias [V]	Noninteracting	STD	LOE
± 0.5	$8 \cdot 10^6$	5	20
± 0.6	$7 \cdot 10^7$	58	200

Timings :

	Noninteracting	STD	LOE
Time spent on IV curve:	28 h	129 h	468 h

- Note that the LOE method requires the calculation of the Hamiltonian derivatives, which is very memory-demanding, and thus impractical for large systems.

https://docs.quantumwise.com/casestudies/std_transport/std_transport.html

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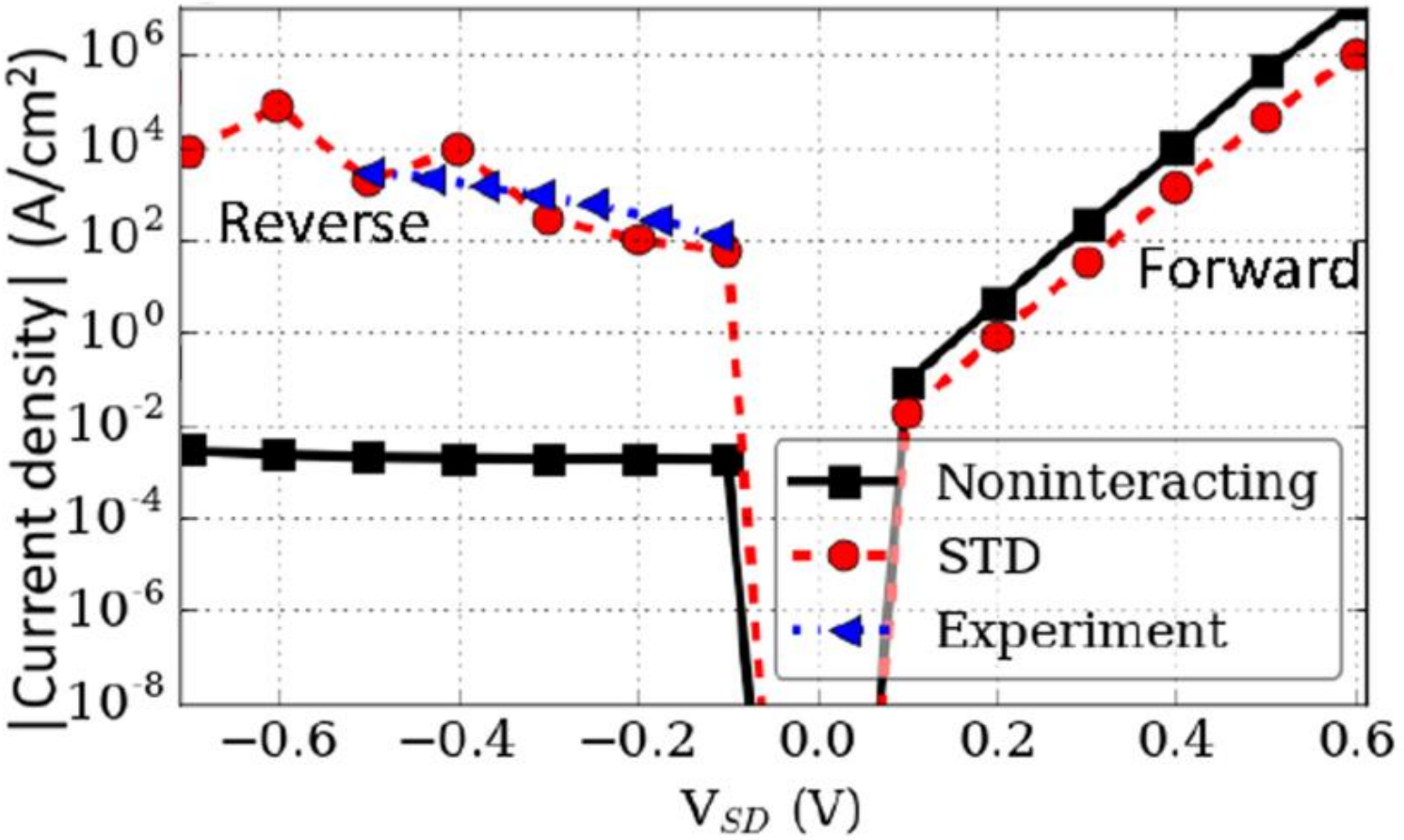
Longer silicon pn-junction also possible – using STD

- This device is 19.6 nm long and 152 atoms
- The previous one is 6.5 nm and 52 atoms
- More advanced methods are unfeasible at this size unless several approximations are used
- Good agreement with experiment



Gunst, T., Markussen, T., Palsgaard, M. L. N., Stokbro, K., & Brandbyge, M. (2017). “First-principles electron transport with phonon coupling: Large scale at low cost.” *Physical Review B*, **96**(16), 161404. DOI: 10.1103/PhysRevB.96.161404

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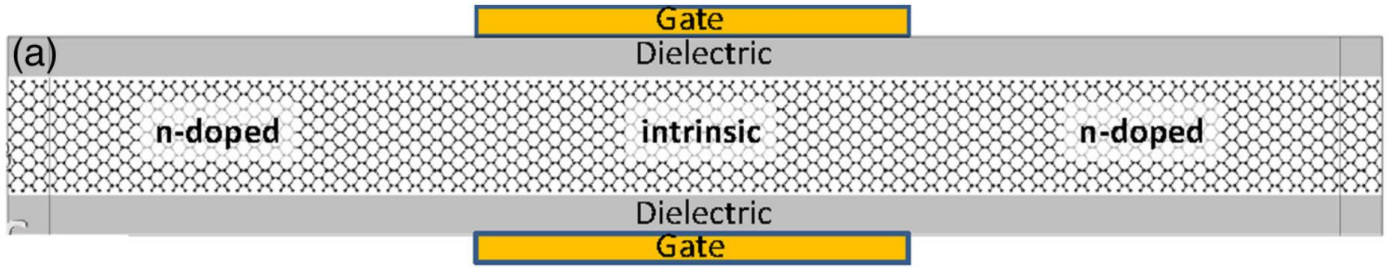
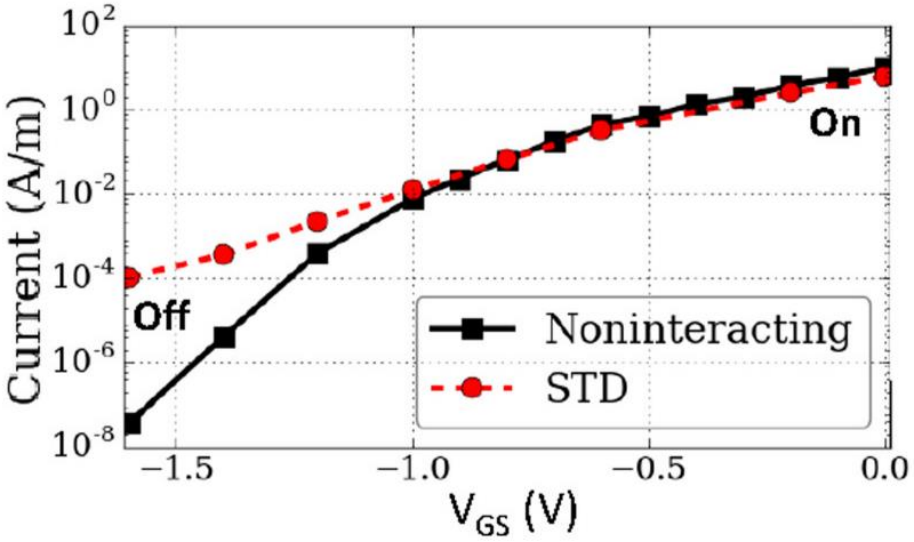
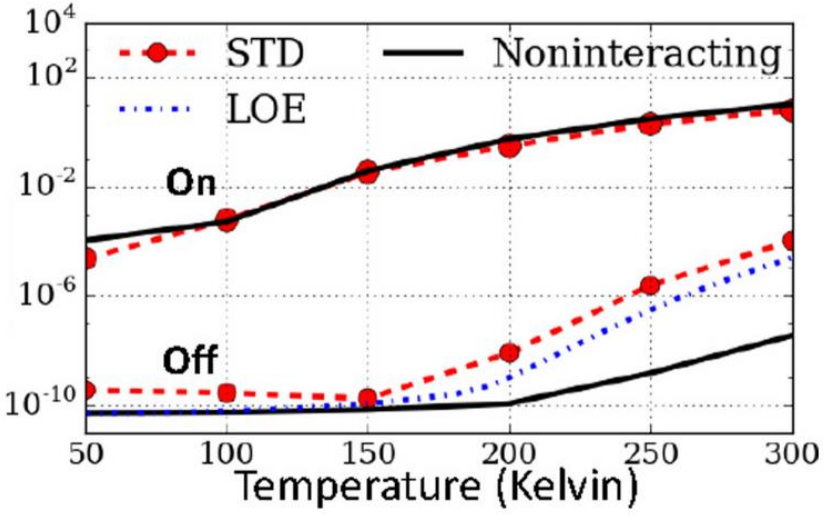
Silicon n-i-n-junction at 300 K – using STD

- Silicon n-i-n junction with a double gate – approximately 30 nm long and 1500 atoms
- Current as a function of gate voltage shows a big impact for the off-state







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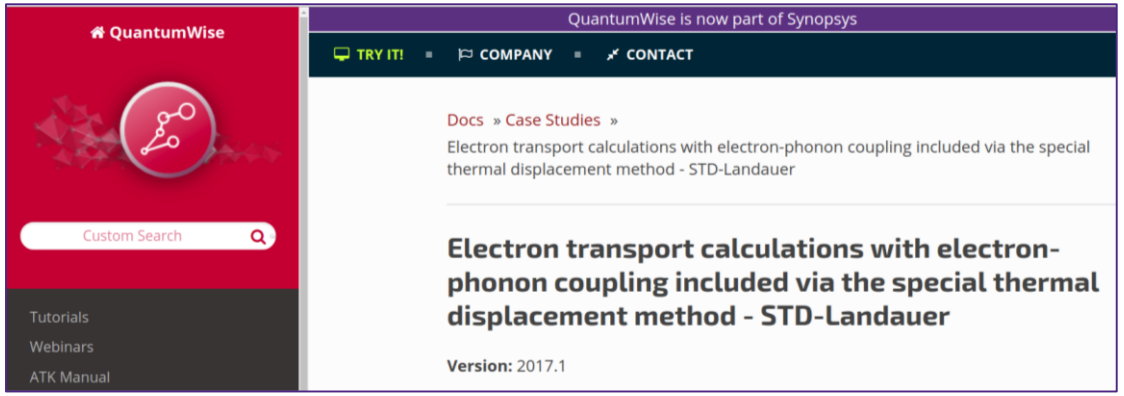
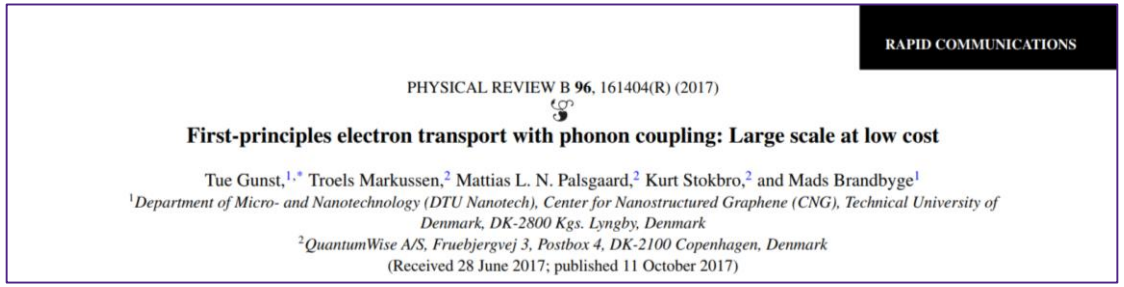
Thank You

Thank You

On-line material:

https://docs.quantumwise.com/casestudies/std_transport/std_transport.html





- ❑ A survey will be sent to all attendees at the end of the webinar