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Resistivity calculations using the MD-Landauer method

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Introduction to QuantumATK
ATK Reference Manual
Transport calculations with QuantumATK

The bulk resistivity is an intrinsic property quantifying how strongly a material disrupts a flux of electronic current. In pristine metals, the main cause of the resistivity at room temperature is electron-phonon interaction, i.e., electron scattering due to the interaction with the vibrations of the lattice. The higher the temperature, the larger becomes the vibrational amplitude of the lattice and hence the scattering probability, leading to linear increase of the resisitivity to the temperature.

This case study aims at introducing the **MD-Landauer** method, which is a conceptually simple methodology for calculating the temperature-dependent resistivity based on combined molecular-dynamics (MD) and electronic-transport calculations within the framework of the Landauer formalism (check the tutorial Transport calculations with QuantumATK). Despite its simplicity, the MD-Landauer method has several advantages over other more rigorous methods to calculate bulk resistivities (see, e.g., Refs. [1] and [2], and also the tutorial Phonon-limited mobility in graphene using the Boltzmann transport equation), as it takes naturally into account the anharmonic effects in describing lattice vibrations, and is applicable to non-crystalline systems as well.

The case study consists of three sections, through which we reproduce some results for bulk gold recently reported in the paper *"Electron-phonon scattering from Green's function transport combined with Molecular Dynamics: Applications to mobility predictions"* [3]. Section 1. Theory and numerical procedure provides some theoretical and methodological details. Section 2. Calculation setup then describes how to setup an MD-Landauer calculation in **QuantumATK**. Finally, Sec. 3. Data analysis is devoted to explaining how to analyze the data files and compute the resistivity.

> ⓘ **Note**
>
> The numerical parameters employed in the calculations below have been tuned to achieve a

compromise between computational efficiency and accuracy. The results will hence slightly differ from those presented in Ref. [3].
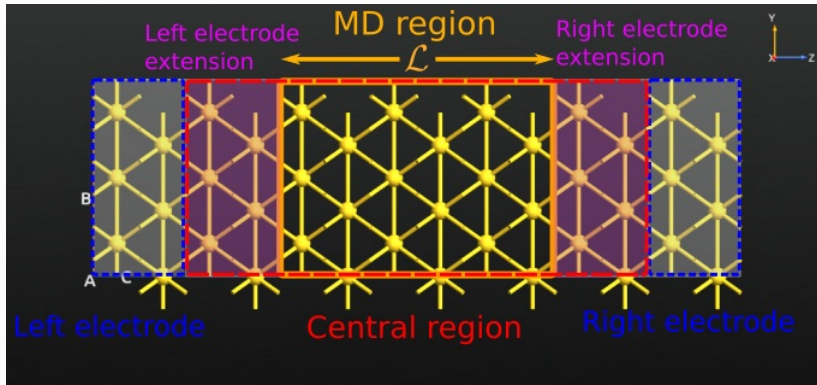
> **❶ Note**
>
> QuantumWise case studies are primarily directed at experienced users of QuantumATK. Instructions are deliberately concise in order to focus mostly on the science.
>
> For more basic details on how to use QuantumATK, please refer to the tutorials Introduction to QuantumATK and Transport calculations with QuantumATK.

1. Theory and numerical procedure

The figure above displays an illustrative example of a device configuration modeling bulk gold, for which the MD-Landauer calculations are performed. There are two semi-infinite electrodes and, in between, a **central region** which, importantly, consists of three parts: the **MD region** with length $\mathcal{L}$ and the **electrode copy** on its either side. An incoming flux of electrons from one of the electrodes interacts with phonons in the MD region, and is transmitted with a certain probability to the other electrode. Assuming that the electrodes and their replicas always remain equilibrium at temperature T, MD calculations are performed by allowing the atoms to move only in the MD region for a few nanoseconds, starting with random initial velocities based on the Maxwell-Boltzmann distribution. At the end of each MD calculations, the transmission coefficient is computed as

$$\mathscr{T}[E; \mathrm{x}(T), \mathcal{L}] = \mathrm{Tr}\big\{G^{\mathrm{r}}[E; \mathrm{x}(T), \mathcal{L}]\Gamma_{\mathrm{L}}(E)G^{\mathrm{a}}[E; \mathrm{x}(T), \mathcal{L}]\Gamma_{\mathrm{R}}(E)\big\},$$

where
$G^{\mathrm{r/a}}[E; \mathrm{x}(T), \mathcal{L}]$ represents the retarded/advanced Green's function, and
$\Gamma_{\mathrm{L/R}}(E)$ is the width in the left/right electrode (see, e.g., Ref. [4] for details of the derivation). Note that the Green's functions and thus the transmission coefficient are both functions of E and parametrically depend on the set of displacement coordinates of atoms $\mathrm{x}(T)$ as well as $\mathcal{L}$. The Landauer formula then provides the conductance as a function of $\mathcal{L}$ and T:

$$\mathscr{G}(\mathcal{L}, T) = \frac{2e^2}{h} \int \langle \mathscr{T}[E; \mathrm{x}(T), \mathcal{L}]\rangle \left[-\frac{\partial n_{\mathrm{F}}(E, \epsilon_{\mathrm{F}}, T)}{\partial E}\right] dE,$$

where
$n_{\mathrm{F}}(E, \epsilon_{\mathrm{F}}, T)$ represents the Fermi-Dirac distribution function with ϵ_{F} being the Fermi energy, and

$\langle \cdots \rangle$ means taking average over a set of MD calculations. The resistance is defined as the inverse of the conductance, i.e.,

$$1/\mathscr{G}(\mathcal{L}, T) = R(\mathcal{L}, T)$$
$$\equiv R_\mathrm{c} + \rho_\mathrm{1D}(T)\mathcal{L},$$

where the second line defines the one-dimensional (1D) resistivity $\rho_\mathrm{1D}(T)$. The bulk resitivity is then given by

$$\rho_\mathrm{bulk}(T) = \rho_\mathrm{1D}(T) \cdot A,$$

where
A is the cross section of the device normal to the transport direction.

Dividing the procedure into three steps as follows will help clarify how to compute the 1D and bulk resistivies:

- **Calculation of the lattice geometries:**

    For a given value of T and a set of values of $\mathcal{L}$, several MD calculations with random initial velocities are performed. For each calculation, the last snapshot of the MD run is taken.

- **Calculation of the resistance:**

    For each set of snapshots with a given length $\mathcal{L}$, the averaged transmission coefficient is computed, which is then used to calculate the conductance $\mathscr{G}(\mathcal{L}, T)$ and the resistance $R(\mathcal{L}, T)$.

- **Calculation of the finite-temperature resistivity:**

    The 1D and bulk resistivities at the temperature T are calculated.

The rest of this case study details each step as well as the procedure to construct a device configuration of bulk gold.
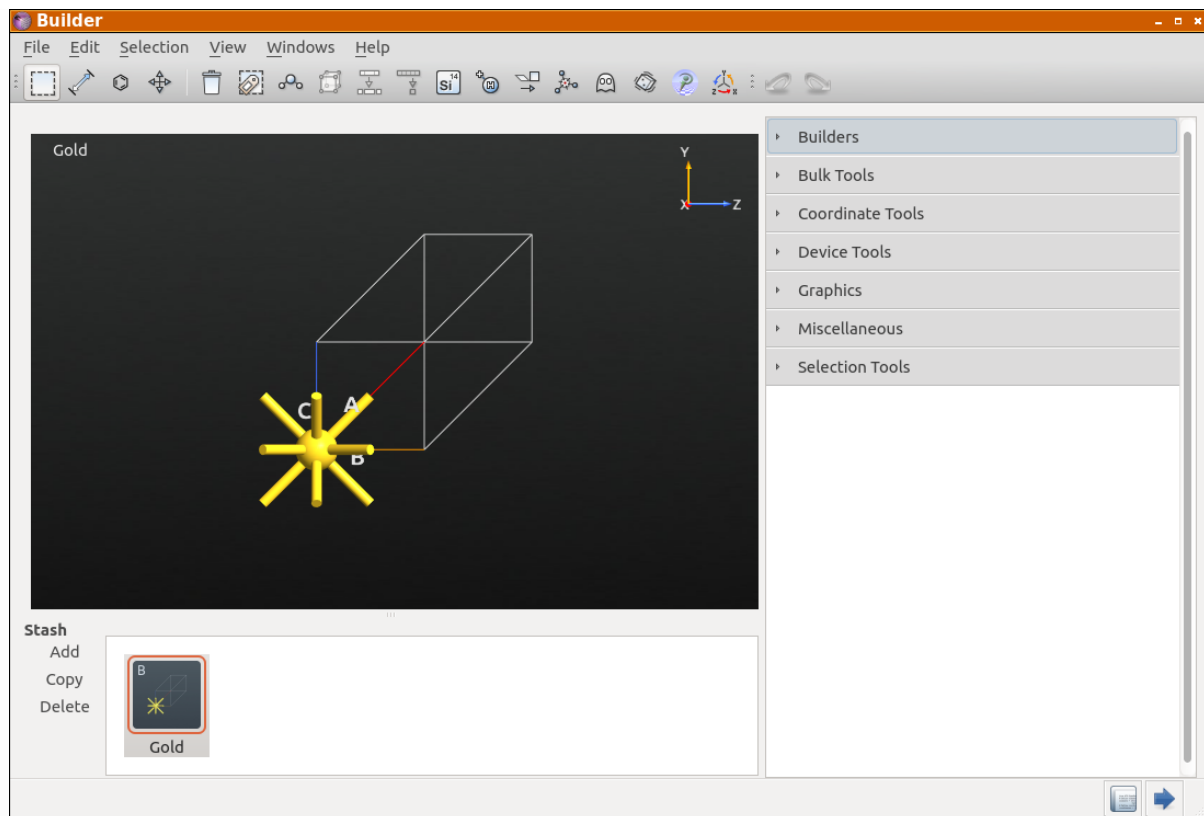
2. Calculation setup

### 2.1. Construction of the DeviceConfiguration

> **❶ Tip**
>
> This subsection presents a detailed how-to guidline for preparing a device configuation of bulk gold, and finally provides an QuantumATK Python script, ⬇ Au100_L3.py. To save time, one may just download the script and use it.

In the 🖉 **Builder**, go to Add ▸ From Database… and select "*Gold*":

Then use the Builders ▸ Surface (Cleave) tool as follows to create a 3x3 Au[100] bulk supercell with a thickness of 10 layers:

1. Create a [100] surface by setting h=0 and k=l=0.
2. Define the surface lattice vectors by

    $v_1 = 3u_1$ and

    $v_2 = 3u_2$.
3. Select "*Periodic and normal (electrode)*" and set the thickness to 10 layers.

(1)

(2)

(3)
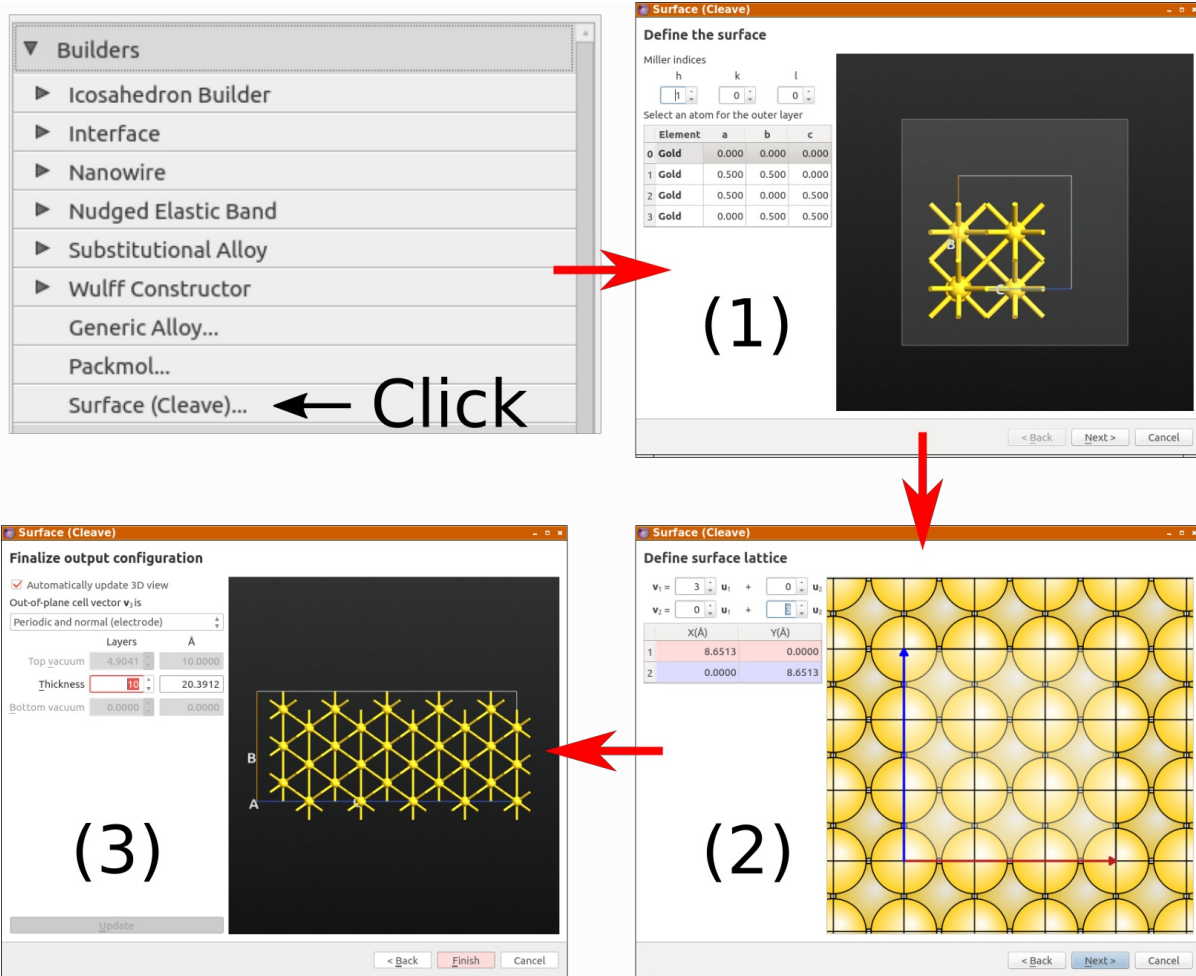
Finally, use the Device Tools ▸ Device from Bulk plugin to create a DeviceConfiguration. Set the length of both right and left electrodes to be the minimum value 4.07825 Å.
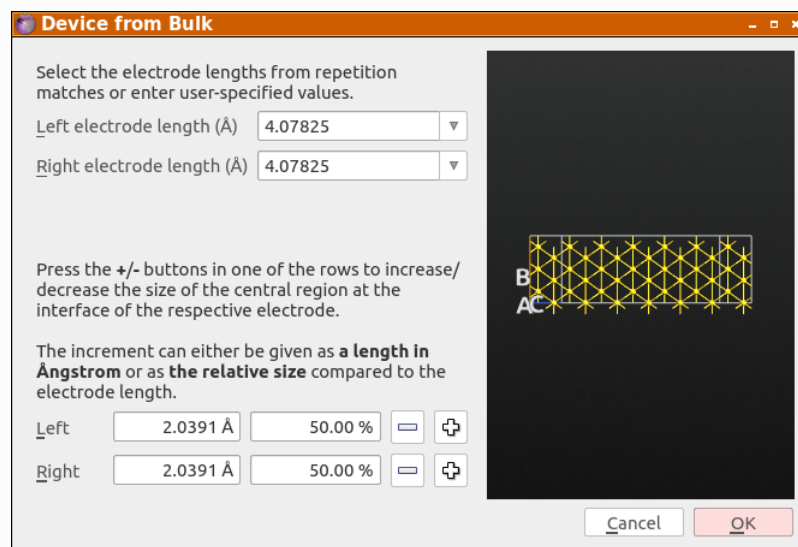

Save the device configuration as "*Au100_L3.py*," where "*L3*" indicates $\mathcal{L} = 3$ in terms of the number of electrode repetitions. Following a similar procedure, one will be able to easily construct the device configurations for $\mathcal{L} = 4$ and 5, and save them with proper file names.

2.2. Setup of the script

Send the device configuration to 🧑 **Scripter** by clicking 🔽 and add four blocks in the order as follows:
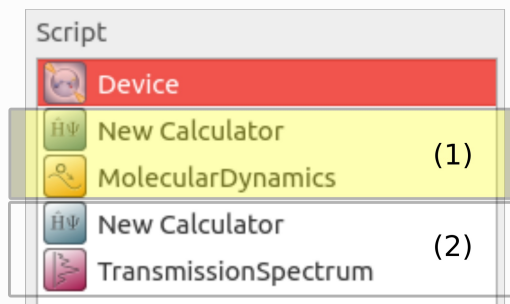
- $\boxed{\hat{H}\Psi}$ New Calculator

- $\boxed{\diagdown}$ Optimization ▸ MolecularDynamics

- $\boxed{\hat{H}\Psi}$ New Calculator

- $\boxed{\diagdown}$ Analysis ▸ TransmissionSpectrum
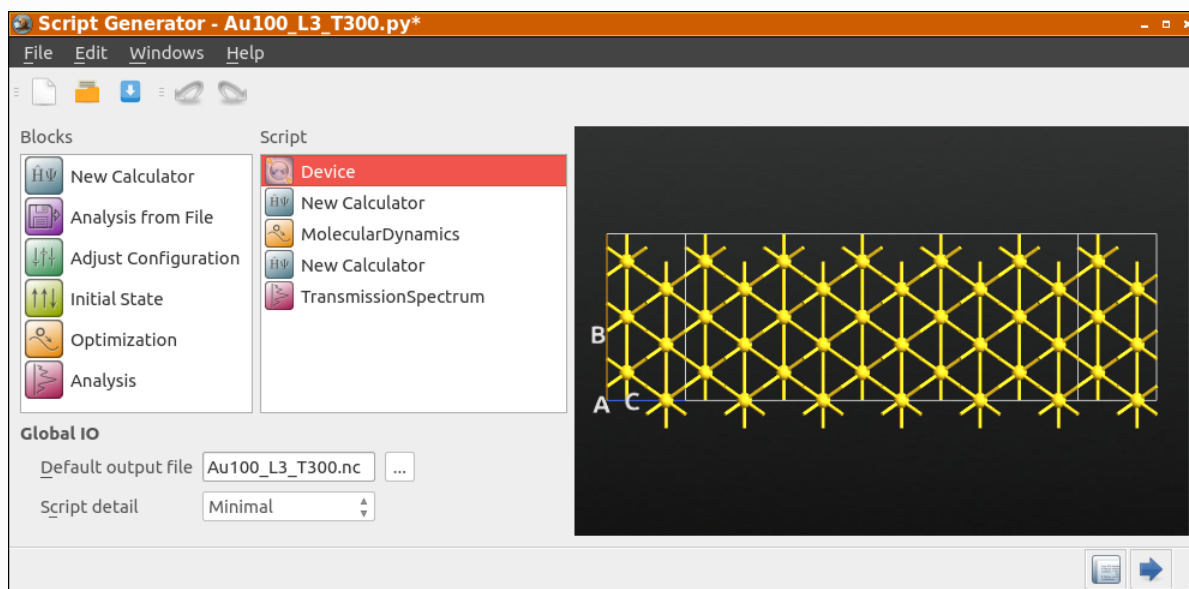
In the section **Global IO options**, change the name of the output file to "*Au100_L3_T300.nc.*" The parameters in each block should then be specified as follow.

MD section

The set of two blocks, $\boxed{\hat{H}\Psi}$ and $\boxed{\diagdown}$, in the section (1) highlighted in yellow, is meant to account for the MD calculations.

Open the $\boxed{\hat{H}\Psi}$ **New Calculator** block, then select ATK-ForceField from the available **Calculators**, and set "*EAM_Au_Sheng_2011*" [5] in **Parameter set**.

In the MolecularDynamics block, choose the Langevin thermostat [6] and set the rest of the MD parameters as shown below.

Landauer calculation section

The set of two blocks, and , in the section (2) highlighted in yellow is meant to account for the DFTB-based transport calculations based on the Landauer approach.
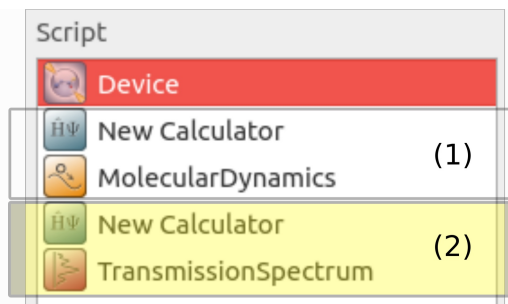
Click on the ⊞ **New Calculator** block. Select "*ATK-SE Slater_Koster (Device)*" from the list of available **Calculators** and set up the parameters as shown below.

❗ Important

Remember to untick "*No SCF iteration*" to carry out the calculations self-consistently.

Click on the 📊 **TransmissionSpectrum** object, and set the parameters as shown below.

Transmission Spectrum

Transmission Spectrum

Energy Range

E_0 (eV) `-0.2`

E_1 (eV) `0.2`

Points `51`

Energy zero parameter `Average Fermi level`

Infinitesimal `1e-06` `eV`

Self-energy calculator `Krylov`

k-point Sampling

Grid type `Monkhorst-Pack grid` `Preset densities ▾`

Periodic ☑ k_A ☑ k_B

○ Density (Å) `13.7689` `13.7689`

◉ Sampling `10` `10` ☐ Sync

Number of symmetry reduced k-points: 15 [Show]

▷ **More options**

IO

☑ Save ☑ Print

File `Au100_L3_T300.nc` `...` Label ` `

[OK]

> **ⓘ Note**
>
> The choice of the "*Krylov*" method is of particular importance as it accelerates the convergence in the SCF calculations.

2.3. Edit the python script

Making fully use of GUI supported by **QuantumATK**, the device configuration has been so far constructed with the necessary calculators and analyzer attached. The MD-Landauer method for computing the conductance, resistance, and resistivity, however, requires performing the calculation, for each of given values of
$\mathcal{L}$ and
T, several times to obtain averaged transmission coefficient
$\langle \mathscr{T}[E; \mathrm{x}(T), \mathcal{L}] \rangle$. To this end, the python script needs to be slightly modified by hand.

By clicking the 🔲 icon, send the script to 🧭 **Editor**. Highlight the whole script and press the `Tab` key on your keyboard to indent every line. Then edit the script as shown below, and save it as "*Au100_L3_T300.py*" To make sure that there is no mistake in your code, download ⬇ Au100_L3_T300.py and compare the two scripts.

```
 1  # -*- coding: utf-8 -*-
 2
 3  for run in range(0,10):
 4
 5      # -------------------------------------------------------------
 6      # Two-probe Configuration
 7      # -------------------------------------------------------------
 8
 9      # -------------------------------------------------------------
10      # Left Electrode
11      # -------------------------------------------------------------
12
13      # Set up lattice
14      vector_a = [8.65127469112, 0.0, 0.0]*Angstrom
15      vector_b = [0.0, 8.65127469112, 0.0]*Angstrom
16      vector_c = [0.0, 0.0, 4.07825]*Angstrom
17      left_electrode_lattice = UnitCell(vector_a, vector_b, vector_c)
```

> **❶ Note**
>
> Since the MD and Landauer sections are all placed under a loop, this script evaluates the transmission coefficient 10 times starting with different values of initial velocity, and saves each result with a unique ID number (gIDxxx) attached.

> **❶ Note**
>
> Following exactly the same procedure except employing different values of
> $\mathcal{L}$, e.g.,
> $\mathcal{L} = 4$ and 5, one can easily prepare the scripts for systematic implementation of the MD-Landauer calculations at
> T =300 K. To save time, one may download ⬇ Au100_L4_T300.py and ⬇ Au100_L5_T300.py, and use them.

3. Data analysis

Click the ⬒ icon, send the script to ⚙ **Job Manager**, and run it. The calculation takes 5-6 hours on 8 cores. The set of transmission coefficients should then be averaged for the analysis. This section hence focuses on how to analyze the results and obtain the 1D and bulk resistivities.

3.1. Transmission functions, conductance, and resistance

QuantumATK provides a useful plugin to make comparison of the transmission functions. Select all the transmission functions $T(\mathbf{k}, \epsilon)$ in **LabFloor** and click the `Compare Data...` button in **Plugin Bar**.
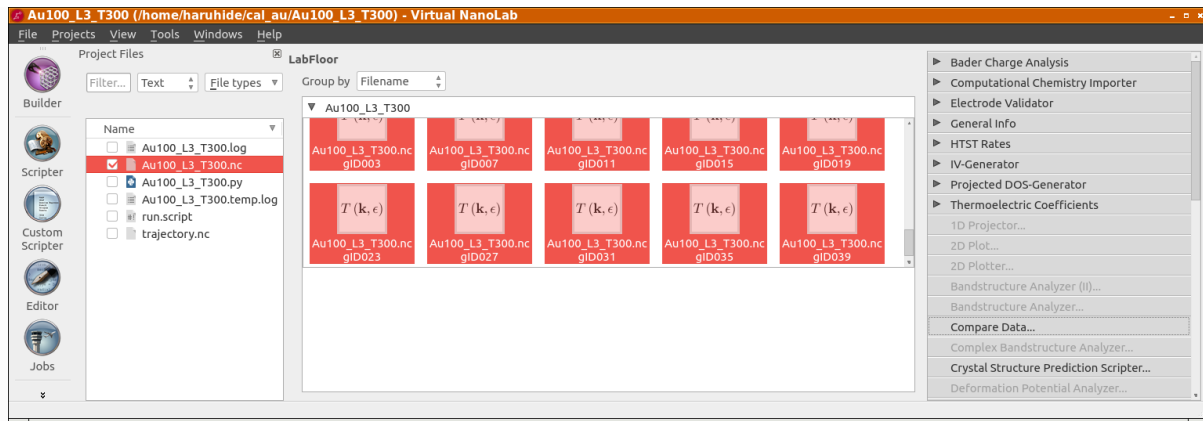
A window will pup up and display all the transmission functions
$$\left\{ \mathscr{T}[E; \mathrm{x}(T), \mathcal{L}] \right\}_{\mathrm{x}(T)} \text{ for}$$
$T = 300$ K and
$\mathcal{L} = 3$.
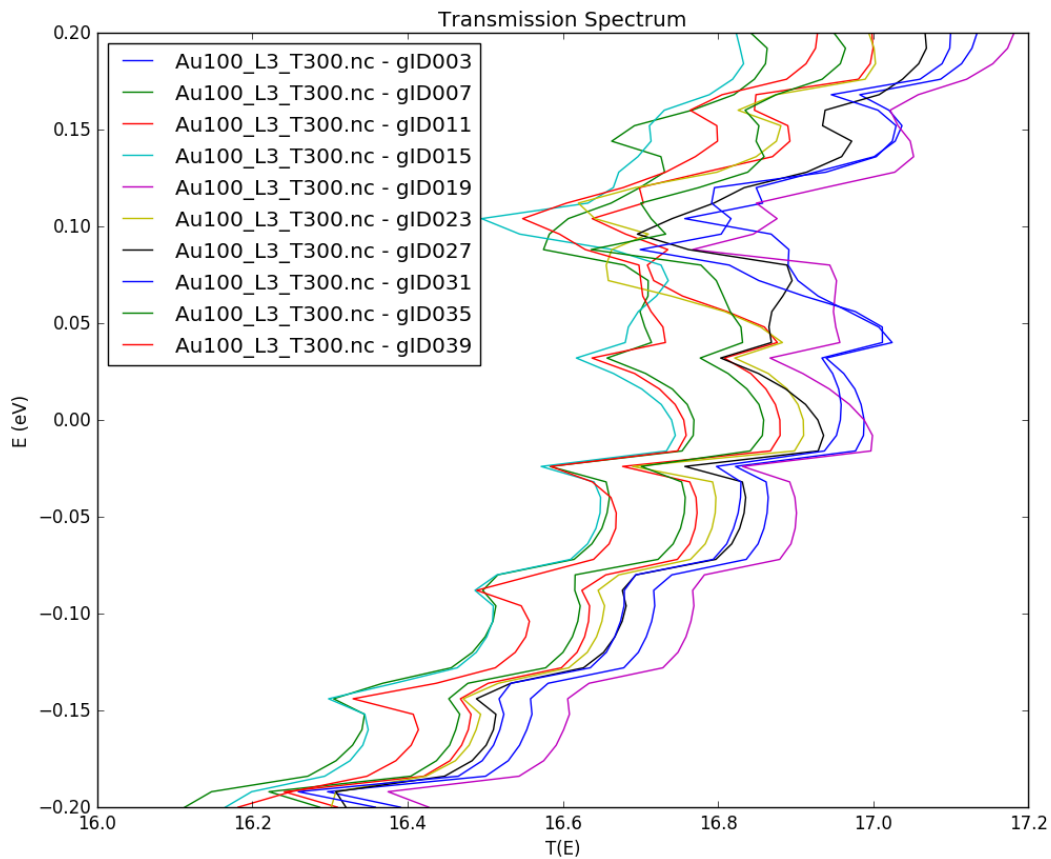
To compute the average of them, download the script ⬇ analysis.py and run it as `atkpython analysis.py` in the same directory of the nc. The analysis will finish in a few seconds, and provide a list of information about the length of the MD-region, and the averaged conductance and resistance:

```
 >_ LXTerminal                                                          _ □ ×
 File  Edit  Tabs  Help
Calculating Kinetic Matrix : =================================================

+--------------------------------------------------------------------+
| MD-Landauer Reprot                                                 |
+--------------------------------------------------------------------+
| Lenght of the MD region = 12.23475 Ang                             |
| Averaged conductance    = 0.000651443815697 Siemens                |
| Averaged resistance     = 1535.05179711 Ohm                        |
+--------------------------------------------------------------------+

Timing:                          Total      Per Step       %

---------------------------------------------------------------------

File IO, nlread        :         1.16 s       0.10 s    25.39% |=============|
Loading Modules + MPI  :         1.07 s       1.07 s    23.29% |============|
---------------------------------------------------------------------
Total                  :         4.59 s
```
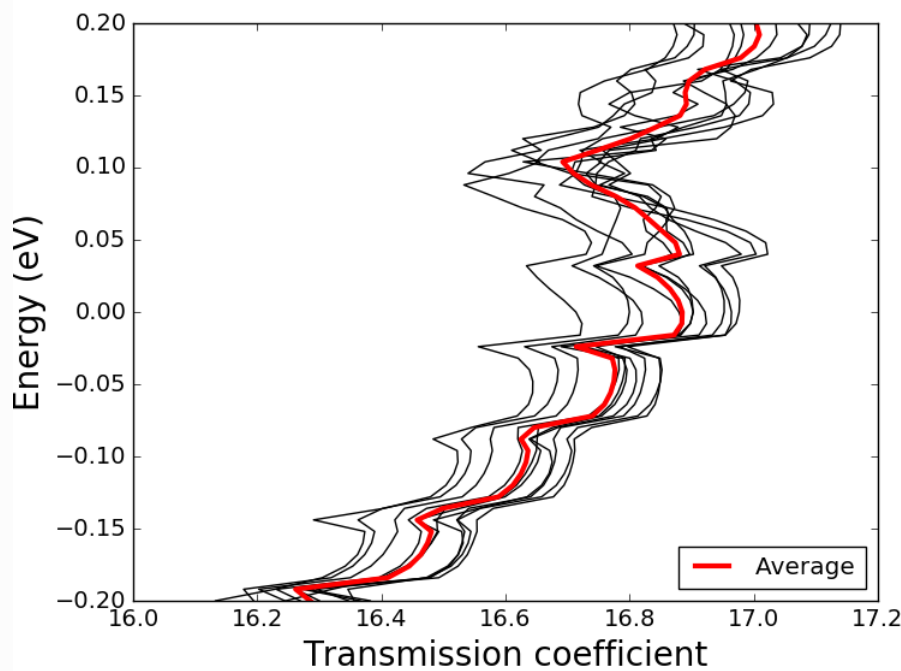
There also appears a pup-up window, in which black lines show the transmission coefficients as before, and a thick red line represents their average $\langle \mathscr{T}[E; \mathrm{x}(T), \mathcal{L}] \rangle$.

3.2. Resistivity

To compute the resistance at $T = 300$ K also for $\mathcal{L} = 0$, 4, and 5, download the scripts ⬇ Au100_L0_T0.py, ⬇ Au100_L4_T300.py, and ⬇ Au100_L5_T300.py. Run them as `atkpython Au100_Lx_Txxx.py`, and analyze the results. One will then obtain a list of resistances, indicating the linear dependence of the resistance on $\mathcal{L}$:

Length of the MD-region, $\mathcal{L}$		Resistance
(# of electrode repetitions)	(Å)	(Ω)
0	0	1482.9
3	12.235	1535.1

Length of the MD-region,		Resistance
4	16.313	1555.2
5	20.391	1571.9

> **❶ Note**
>
> The resistance for
> $\mathcal{L} = 0$ is computed using the script ⬇ Au100_L0_T0.py, which implements no MD calculation, and because of it, is hence named with "*T0*." This script aims at evaluating the contact resistance.

Let us then compute the 1D and bulk resistivities, which requires the value of the cross section. Noting the primitive vectors defined in lines 14 and 15 of "*Au100_L3_T300.py*," i.e.,

```
14    vector_a = [8.65127469112, 0.0, 0.0]*Angstrom
15    vector_b = [0.0, 8.65127469112, 0.0]*Angstrom
```

the cross section, in this case, is given by
$A =$
$\|$vector_a
$\| \times$
$\|$vector_b
$\| = 74.84$ Å
^{2}. Using this value, and also the values of
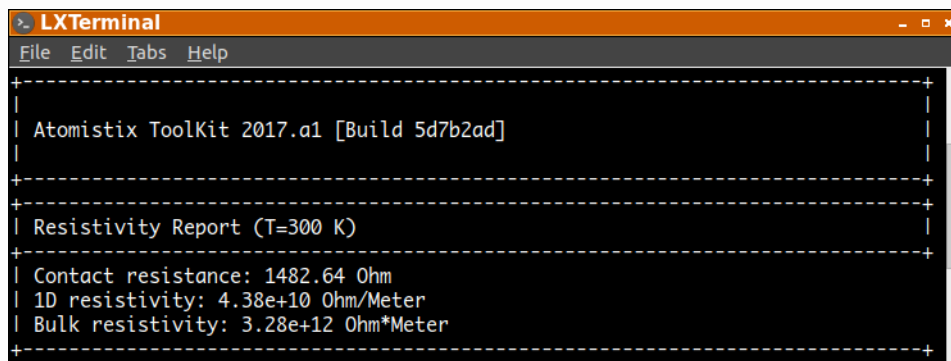$\mathcal{L}$ and resistance listed in the table above, one can evaluate the 1D and bulk resistivities at
$T = 300$ K. To this end, download ⬇ resistivity.py, and, after entering the values in the table into the
**INPUT SECTION** of the script, run it as `atkpython resistivity.py`.

```
 6 #------------------------------------------------------------------#
 7 #                        INPUT SECTION                             |
 8 #------------------------------------------------------------------#
 9 cs_area = 8.65127469112**2
10 lengths_list = [0,12.235,16.313,20.391]
11 resistances_list = [1482.9,1535.1,1555.2,1571.90]
12 output_filename = 'resistivity.png'
```

The script interpolates the data points by means of the least squares method and provides the values of the contact resistance, as well as the 1D and bulk resistivities at
$T = 300$ K:

```
LXTerminal                                                  _ □ x
File  Edit  Tabs  Help
+------------------------------------------------------------------+
|                                                                  |
| Atomistix ToolKit 2017.a1 [Build 5d7b2ad]                        |
|                                                                  |
+------------------------------------------------------------------+
+------------------------------------------------------------------+
| Resistivity Report (T=300 K)                                     |
+------------------------------------------------------------------+
| Contact resistance: 1482.64 Ohm                                  |
| 1D resistivity: 4.38e+10 Ohm/Meter                               |
| Bulk resistivity: 3.28e+12 Ohm*Meter                             |
+------------------------------------------------------------------+
```
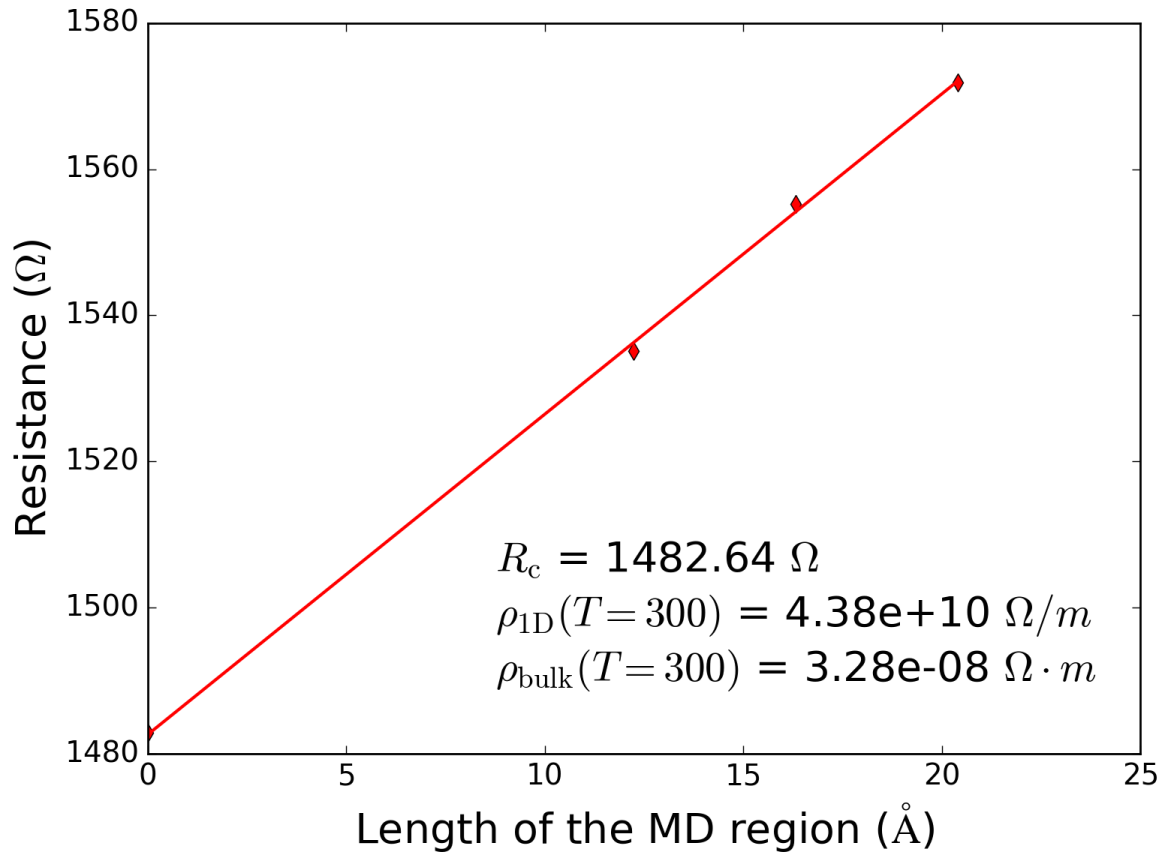
A red diamond in the figure below is the bulk resistivity at
$T = 300$ K, and is compared with purple points representing the results of the MD-Landauer calculations shown in Fig. 7(b) of Ref. [7]. Because of the reduced numerical condition employed in this case study, there exists a small difference. The figure also displays black squares representing the experimental result [7], and proves the qualitative agreement with the MD-Landauer result.
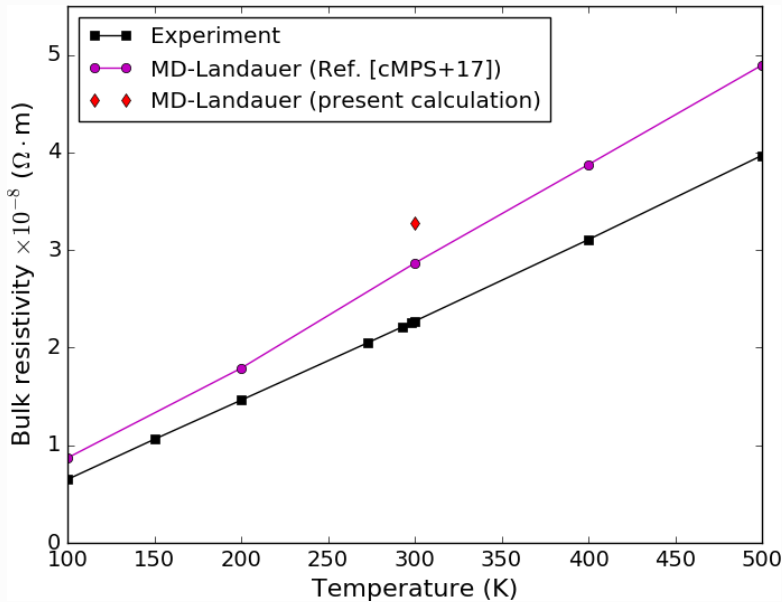
References

[1]
M. Brandbyge, J.-L. Mozos, P. Ordejón, J. Taylor, and K. Stokbro. Density-functional method for nonequilibrium electron transport. *Phys. Rev. B*, 65:165401, Mar 2002. doi:10.1103/PhysRevB.65.165401.

[2]
K. Stokbro, D. E. Petersen, S. Smidstrup, A. Blom, M. Ipsen, and K. Kaasbjerg. Semiempirical model for nanoscale device simulations. *Phys. Rev. B*, 82:075420, Aug 2010. doi:10.1103/PhysRevB.82.075420.

[3] (1,2)
T. Markussen, M. Palsgaard, D. Stradi, T. Gunst, M. Brandbyge, and K. Stokbro. Electron-phonon scattering from green's function transport combined with molecular dynamics: applications to mobility predictions. *Phys. Rev. B*, 95:245210, June 2017. URL: https://arxiv.org/abs/1701.02883, doi:10.1103/PhysRevB.95.245210.

[4]
S. Datta. *Electronic Transport in Mesoscopic Systems*. Cambridge University Press, 1997. ISBN 0521599431. Cambridge Studies in Semiconductor Physics and Microelectronic Engineering.

[5]
H. W. Sheng, M. J. Kramer, A. Cadien, T. Fujita, and M. W. Chen. Highly optimized embedded-atom-method potentials for fourteen fcc metals. *Phys. Rev. B*, 83:134118, April 2011. doi:10.1103/PhysRevB.83.134118.

[6]
N. Goga, A. J. Rzepiela, A. H. de Vries, S. J. Marrink, and H. J. C. Berendsen. Efficient algorithms for langevin and dpd dynamics. *Journal of Chemical Theory and Computation*, 8(10):3637−3649, 2012. PMID: 26593009. doi:10.1021/ct3000876.

[7] (1,2)
D. R. Lide. *Handbook of Chemistry and Physics*. New York: CRC Press, 75th edition, 1997.