Geometry optimization of interfaces

In this tutorial you will learn how to setup and optimize the geometry of interfaces for 2-probe device calculations.

You will use the VNL Interface Builder, and learn how to use a combination of “rigid” constraints and a simple optimization algorithm to perform efficient and reliable relaxation of the internal coordinates in a device configuration.

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### Building blocks of an interface

- **Electrode**
- **Extension**
- **Scattering region**
- **Central region**

- **Probe A**
- **Probe B**

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### In details: step-by-step optimization process

#### A. Bulk Rigid Optimization (BRO) of the regions A2+3 and B2+3

- Using DFT, classical potential, DFTB...
- Fully relaxed

#### B. Scattering Region Bulk Optimization (SRBO) of the regions A3 and B3

- A2 and B2 are rigid bodies
- Move in 3D space
- Atoms in A3 and B3 free to relax
- Vacuum relaxation

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### Device 1D Minimization (D-1DMin)

A somewhat more brute-force approach is to explicitly minimize the device total energy w.r.t. internal coordinates and the scattering region length. Namely, do the full 2-probe calculations and vary the scattering region length, while the atoms in A3 and B3 are allowed to relax.

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### QuantumWise

QuantumWise develops commercial software for fast and reliable atomic-scale modeling of nanostructures, fully supported and delivered in an easy-to-use interface, tailored from state-of-the-art methods, and developed by experts to the specifications of our customers.

Atomistix ToolKit (ATK) offers unique capabilities for simulating atomic-scale systems. Based on an open architecture which integrates a powerful scripting language with a graphical user interface.

Virtual NanoLab (VNL) works as a graphical user interface for ATK, but QuantumWise also develops extendable tools allowing VNL to act as a flexible GUI for other software packages apart from ATK.