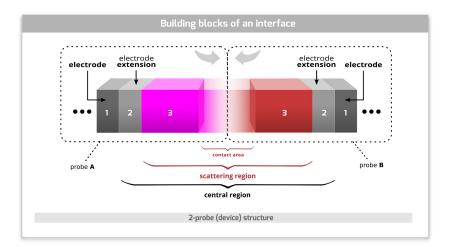
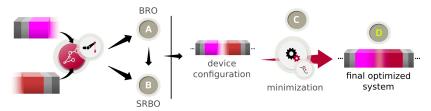
Geometry optimization of interfaces

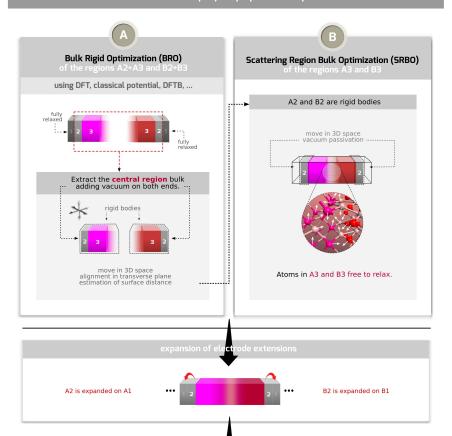
In this tutorial you will learn how to setup and optimize the geometry of interfaces for 2-probe device calculations.

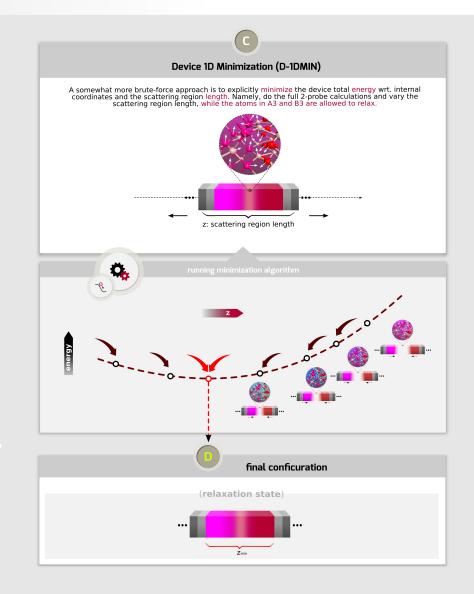
You will use the VNL Interface Builder, and learn how to use a combination of "rigid" constraints and a simple optimization algorithm to perform efficient and reliable relaxation of the internal coordinates in a device configuration.





.. in details: step-by-step optimization process





- Note:

 The geometry of each region should be *separately optimized* in a first-principles manner.

 Both electrode extensions in the central region must *always match* the corresponding electrode.

 The optimum length of the central region is usually not known a *priori*.

 - We rely on minimizing the device total energy while explicitly preserving the internal coordinates
 of the electrode extensions.





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