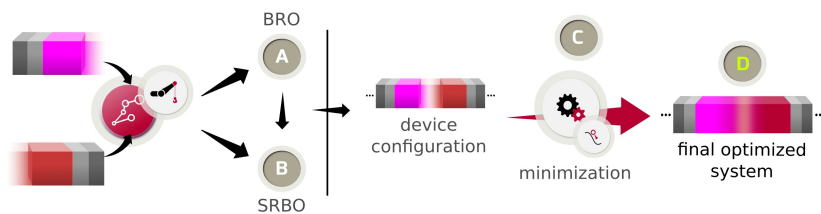


In this tutorial you will learn how to setup and optimize the geometry of interfaces for 2-probe device calculations.

Building blocks of an interface



A

using DFT, classical potential, DFTB, ...



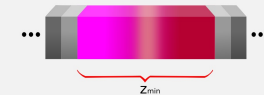
A2 and B2 are rigid bodies



A2 is expanded on A1

B2 is expanded on B1

(relaxation state)



MEMO —

Quantum Wise

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.