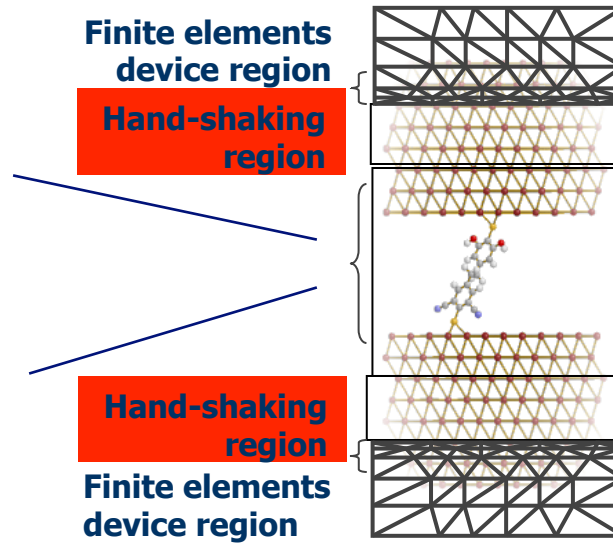
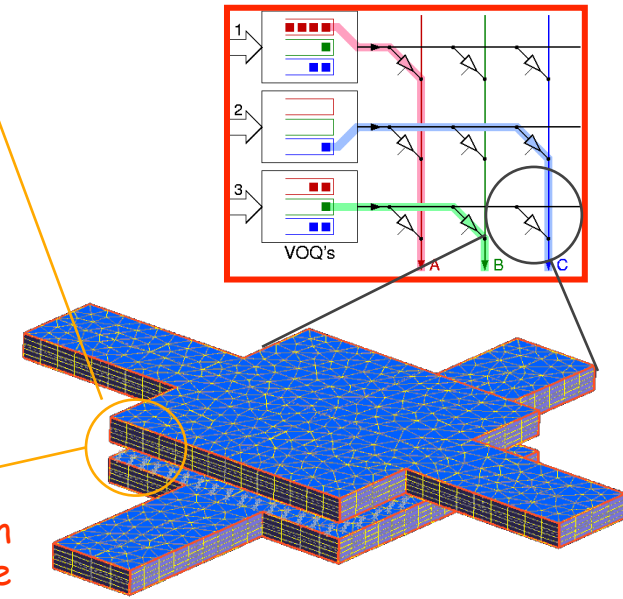


DFTB + quantum-transport approaches using Non-equilibrium Green Functions.



Well-established drift diffusion simulator codes are used to simulate contacts and devices surrounding the molecules.



Circuit level

nanometer region

submicron to micron region

Micron to millimeter regions

Ab initio models

Quantum-classical interfaces

Continuum-based and circuit models

Physics/Chemistry

Engineering