The following page (in construction) describes the simulation of devices with open boundary conditions such as RTDs with the nextnano.NEGF software.

Note that in the current version (2022-03-30), only single band calculations are supported for open boundary conditions. A multiband version is currently developed.

Simulation of devices with open boundary conditions

In order to simulate a system with open boundary conditions (instead of the default field-periodic boundary condition), contacts have to be defined by adding a <Contacts> section in the input file:

```
<Contacts>
   <DensityLeft unit="cm^-3">1e18</DensityLeft>
   <DensityRight unit="cm^-3">1e18</DensityRight>
   <MaterialLeft>well</MaterialLeft>
   <MaterialRight>well</MaterialRight>

   <Broadening unit="meV">10.0</Broadening>
   <Ballistic>no</Ballistic>
</Contacts>
```

In this section, the carrier densities in the left and right contact have to been defined using the <DensityLeft> and <DensityRight> commands, as shown above. The unit is cm^{-3}.

The material of the left and right contacts needs to be defined by te command <MaterialLeft> and <MaterialRight>. The string value has to be an alias defined in the <Materials> section of the input file.

A broadening energy can be defined by the command <Broadening>. Indeed, scattering is not accounted in the contact, so that this commands allows a phenomenological broadening of the density of states in the contact.

The command <Ballistic> can be used to calculate ballistic transport between the contacts (i.e. no scattering process considered) if its value is set to yes.

The tutorial for AlGaAs/GaAs intraband RTD is available on our new manual from here.

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