

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 (2020-06-18), only single band calculations are supported for such open boundary conditions.

## 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 contact have to be defined using the <DensityLeft> and <DensityRight> commands, as shown above. The unit is  $\text{cm}^{-3}$ .

From:

<https://nextnano-docu.northeurope.cloudapp.azure.com/dokuwiki/> - nextnano.NEGF - Software for Quantum Transport

Permanent link:

[https://nextnano-docu.northeurope.cloudapp.azure.com/dokuwiki/doku.php?id=qcl:simulation\\_of\\_resonant\\_tunneling\\_diodes\\_rtds&rev=1592575312](https://nextnano-docu.northeurope.cloudapp.azure.com/dokuwiki/doku.php?id=qcl:simulation_of_resonant_tunneling_diodes_rtds&rev=1592575312)

Last update: 2020/06/19 15:01