

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, 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 cm^{-3} .

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