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 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 strong value has to be an alias defined in the <Materials> section of the input file.