Advanced settings

Parallelization

The number of threads can be controlled using the command <Maximum_Number_of_Threads>

```
<Simulation_Parameter>
  ...
  <Maximum_Number_of_Threads>12</Maximum_Number_of_Threads>
  ...
</Simulation_Parameter>
```

For optimal performances, we recommended that <Maximum_Number_of_Threads> does not exceed the number of **physical** cores (when hyperthreading is activated, the number of physical cores is half the one on logical processsors).

Parallelization in case of combined Temperature-Voltage sweep

In the case where a combined Temperature-Voltage sweep is used, there are two levels of parallelization. The first is at the level of the command <Threads> in the <SweepParameters> section.

```
<SweepParameters>
  <SweepType>Temperature-Voltage</SweepType>
  ...
 <Threads>6</Threads> <!-- Parallelization for Temperature-Voltage sweep -->
 </SweepParameters>
```

The second level of parallelization occurs in the <Simulation_Parameter> section:

```
<Simulation_Parameter>
  ...
  <Maximum_Number_of_Threads>2</Maximum_Number_of_Threads>
  ...
</Simulation_Parameter>
```

In this example, the total number of threads will be <Threads>* <Maximum_Number_of_Threads> = 6*2 = 12.

Scattering processes

Contributions of individual scattering processes

The following command allow to display self-energies and spectral functions for some specific

mechanisms, like e.g. scattering due to optical phonons:

```
<Scattering>
  ...
  <Separate_Scattering>yes</Separate_Scattering>
  ...
</Scattering>
```

This command is only for analysis purpose, and has no influence on the other calculated quantities. It only involves an additionnal calculation of self-energies and Green's functions. In each basis folder, a folder with the name of the scattering process will appear, containing the retarded self-energy and the spectral function arising only from the specific scattering mechanism. Hence this spectral function gives the contribution to broadening of an individual scattering process.

Homogeneous Coulomb scattering

To speed up the calculation, it is possible to consider the assumption of homogeneously distributed Coulomb scatterers (ionized impurities and other charge carriers) using the following command:

```
<Scattering>
  ...
  <Homogeneous_Coulomb>yes</Homogeneous_Coulomb>
  ...
</Scattering>
```

Output format for 2D plots

By default, 2D plots are output in a VTK format (.vtr extension). Gnuplot files (.plt extension) are also generated (in a file explorer, double click on the file to generate the gnuplot figure).

In addition, to output 2D plots in a AVS/Express format (.fld extension), the following command "<FLD_format>" can be added in the <Output> section of the input file.

The following commands can be used to control the output formats:

```
<Output>
...
<VTK_format>yes</VTK_format>
<FLD_format>yes</FLD_format>
<Gnuplot_format>yes</Gnuplot_format>
...
</Output>
```

Scaling 1D wavefunctions

In order to scale the output of the square of the wavefunctions (1D plots), the following command can be used:

```
<Output>
...
<ScaleWaveFunction>0.1</ScaleWaveFunction>
...
</Output>
```