The nextnano.NEGF software for Quantum Transport

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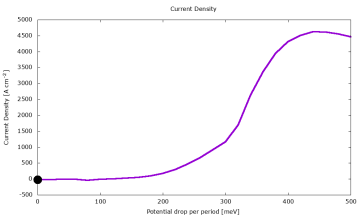
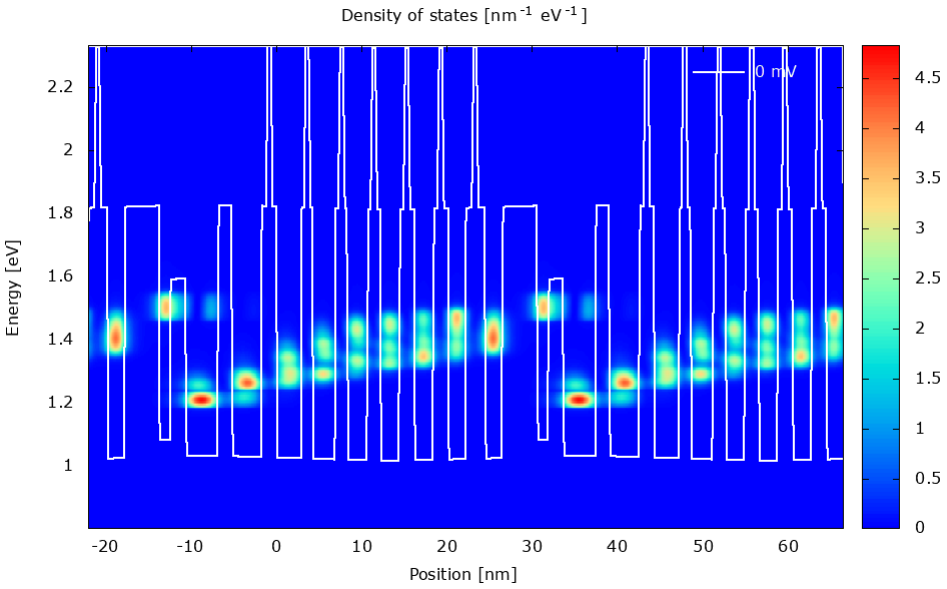
This website describes the nextnano.NEGF software (previously called nextnano.QCL), a **NEGF quantum transport code** written by Thomas Grange. The nextnano.NEGF software has been developed to simulate electron dynamics in heterostructures like superlattices and **quantum cascade lasers** (QCLs). It can also be used to simulate absorption spectra in quantum wells (QWs) and transport in **resonant tunneling diodes** (RTDs).





The software calculates current-voltage characteristics and gain/absorption spectra.

This software is based on a quantum transport method that follows the **nonequilibrium Green's function** (NEGF) framework. The code can be executed using the nextnanomat software.

Which scattering mechanisms are included?

- Longitudinal polar-optical phonon scattering (polar LO phonon scattering)
- Acoustic phonon scattering
- Charged impurity scattering
- Interface roughness scattering
- Alloy scattering
- Electron-electron scattering

How do I obtain the nextnano.NEGF code?

Please download it from here. Additionally, it is strongly recommend to contact

support@nextnano.com and inform us that you are interested in this tool. We can then assist you and provide new updates to you.

How do I execute nextnano.NEGF?

Open the nextnanomat GUI, open a nextnano.NEGF input file and press the Run button.

How do I execute nextnano.NEGF from the command line? (not recommended)

```
nextnano.NEGF.exe <input file name> <output folder name> <material database name> <License file name>
```

Example:
```
./nextnano.NEGF.exe "..\nextnano.NEGF sample files\MidIR_QCL_YuSlivkenRazeghi_SST2010.xml" "..\Output" "..\Material_Database.xml" "..\License_nnQCL.lic"
```

Optional: the argument “–threads 2” can be appended to the command line to limit the number of threads to e.g. 2.

Are there any tutorial input files available?

Various sample files are distributed with the software, including Mid-IR QCLs, THz QCLs and RTDs. The syntax of the input file is explained here.

Where can I find some background on the implemented physics?

The NEGF method for QCLs is decribed in the following publications where the nextnano.NEGF code was used.

- Contrasting influence of charged impurities on transport and gain in terahertz quantum cascade lasers
  T. Grange
  Physical Review B 92, 241306(R) (2015)
- Nanowire terahertz quantum cascade lasers
  T. Grange
  Applied Physics Letters 105, 141105 (2014)
- Electron transport in quantum wire superlattices
  T. Grange
  Physical Review B 89, 165310 (2014)
- Room temperature operation of n-type Ge/SiGe terahertz quantum cascade lasers predicted by non-equilibrium Green's functions

Thomas Grange, David Stark, Giacomo Scalari, Jérôme Faist, Luca Persichetti, Luciana Di Gaspare, Monica De Seta, Michele Ortolani, Douglas J Paul, Giovanni Capellini, Stefan Birner, and Michele Virgilio
Applied Physics Letters 114, 111102 (2019) arXiv

- Atomic-Scale Insights into Semiconductor Heterostructures: From Experimental Three-Dimensional Analysis of the Interface to a Generalized Theory of Interfacial Roughness Scattering
  T. Grange, S. Mukherjee, G. Capellini, M. Montanari, L. Persichetti, L. Di Gaspare, S. Birner, A. Attiaoui, O. Moutanabbir, M. Virgilio, and M. De Seta
  Phys. Rev. Applied 13, 044062 (2020) arXiv

A good introduction is also the tutorial talk Modeling electron transport in quantum cascade lasers given by Thomas Grange at the International Quantum Cascade Laser School and Workshop (Cassis/France, 2018).

The following online presentations are related to the physics implemented in the nextnano.NEGF software:

- Atomic-scale modeling of interface roughness scattering in Quantum Cascade Lasers was given as in invited talk of the Photonics West Conference 2021.
- Microscopic modeling of interface roughness scattering in quantum cascade lasers was given as in invited talk of the | NUSOD conference 2022.

Copyright information

The nextnano.NEGF software has been developed by Thomas Grange. It is written in C#. For publications of Thomas Grange, see his profile on Google Scholar.

The nextnano.NEGF software is distributed by the nextnano GmbH.

For questions or feedback about the software, please contact support@nextnano.com.

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