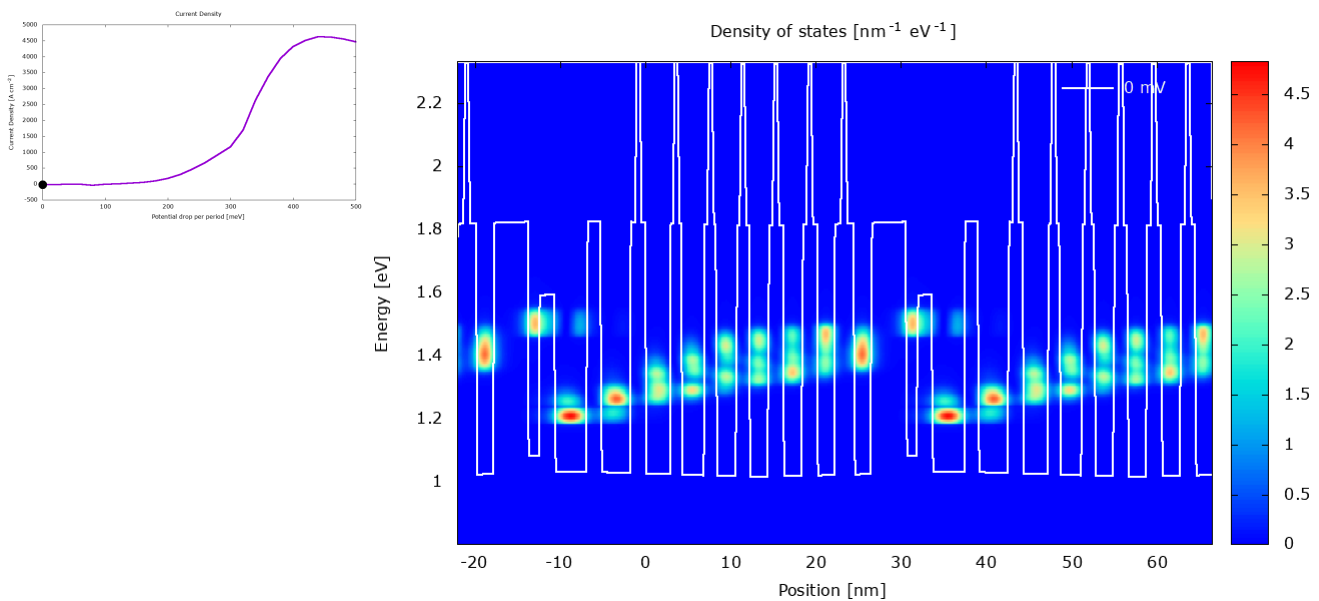


The nextnano.NEGF software for Quantum Transport

- [Getting started](#)
- [Download nextnano.NEGF software](#)
- [License activation](#)

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?

- [Tutorial - GaAs/AlGaAs THz QCL](#)
Terahertz quantum cascade lasers operating up to ~ 200 K with optimized oscillator strength and improved injection tunneling
S. Fatholouloumi, E. Dupont, C.W.I. Chan, Z.R. Wasilewski, S.R. Laframboise, D. Ban, A. Mátyás, C. Jirauschek, Q. Hu, H. C. Liu
Optics Express 20, 3866 (2012)
- [Tutorial - InGaAs/InAlAs Mid-IR QCL](#)
Injector doping level-dependent continuous-wave operation of InP-based QCLs at $\lambda = 7.3 \mu\text{m}$ above room temperature
J. S. Yu, S. Slivken, M. Razeghi
Semiconductor Science and Technology 25, 125015 (2010)

Further tutorials can be found here: [Tutorials](#)

Where can I find some background on the implemented physics?

The NEGF method for QCLs is described 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 online presentation on [Atomic-scale modeling of interface roughness scattering in Quantum Cascade Lasers](#) was given as an invited talk of the Photonics West Conference 2021.

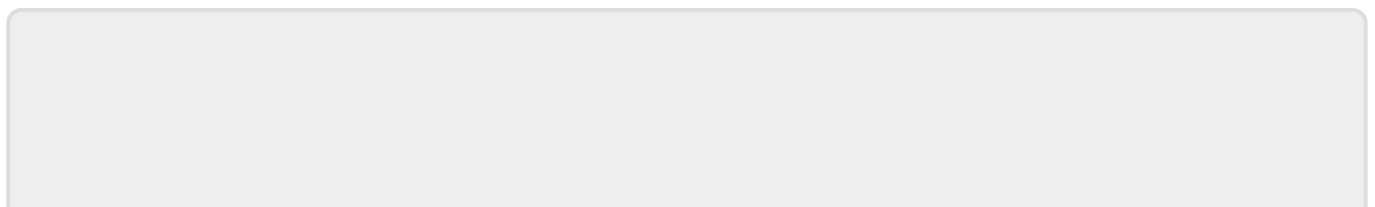
Copyright information

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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