

# Simulation of semiconductor nanodevices with the nextnano software

**Stefan Birner**<sup>1</sup>

<sup>1</sup>*nextnano GmbH, 85586 Poing, Germany*

The commercial nextnano software [1] is a semiconductor nanodevice simulation tool that has been developed for predicting and understanding a wide range of electronic and optical properties of quantum structures. The underlying idea is to provide a robust and generic framework for modeling device applications in the field of nanosized semiconductor heterostructures (quantum wells, wires and dots). The simulator deals with realistic geometries and any combination of materials in one, two, and three spatial dimensions. It focuses on an accurate and reliable treatment of quantum mechanical effects and provides a self-consistent solution of the Schrödinger, Poisson, and current equations. The electronic structure is represented within the single-band or multiband  $k \cdot p$  envelope function approximation, including magnetic field, strain, piezo and pyroelectric fields, and arbitrary crystallographic growth directions. The user interface simplifies running repetitive tasks such as parameter sweeps. The material database includes binaries, ternaries and quaternaries of group IV, III-V and II-VI materials in both zinc blende and wurtzite crystal structure. More recently, the software has been integrated into a Python workflow allowing for automatic optimization of device designs.

In this contribution, we give an overview of the nextnano software and present typical examples that demonstrate the wide range of possible applications such as LEDs, HEMTs and quantum dots. For modeling transport and gain in Quantum Cascade Lasers, an advanced quantum transport model based on the nonequilibrium Green's function method is used.

The progress of charge manipulation in semiconductor-based nanoscale devices opened up a novel route to realize a flying qubit with a single electron in electrostatically defined quantum point contact geometries. In this contribution we introduce the concept of these flying electron qubits, discuss their most promising realizations in two-dimensional electron gases (2DEGs) and show how numerical simulations are applicable to accelerate experimental development cycles of metallic gate layout optimizations [2, 3].

[1] [www.nextnano.com](http://www.nextnano.com)

[2] Semiconductor-based electron flying qubits: review on recent progress accelerated by numerical modelling, H. Edlbauer et al., EPJ Quantum Technology 9, 21 (2022)  
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