Open-source bandstructure and transport models of semiconductor nanostructures for the Quantum Wells, Wires and Dots (QWWAD) simulation suite

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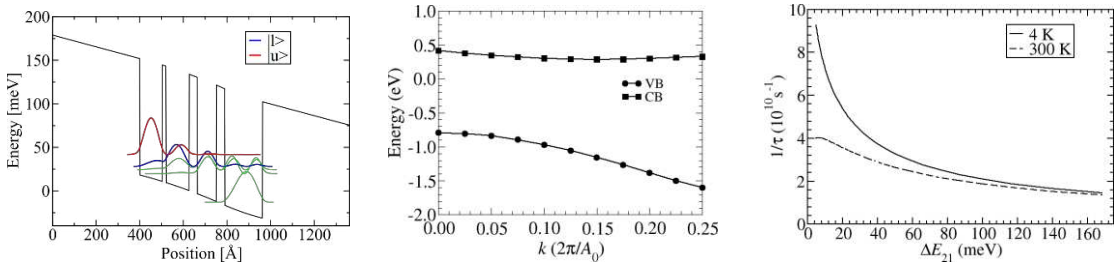
A wide range of high-quality software is available for simulating the band-structure, charge transport and optoelectronic properties of semiconductor nanostructures (e.g., [1]). However, the vast majority is supplied under a proprietary license and its source code cannot be studied, modified or redistributed by its users. The recently created open-source project, *Quantum Wells, Wires and Dots* (QWWAD) [2] is intended as a free, non-commercial community-driven resource, which accompanies the new 4th edition of the eponymous textbook [3]. We describe the new tools for bandstructure and transport modelling that have been included in the latest release (v1.3) in addition to new software infrastructure to enable robust community-led development.



(a) (b) (c)

Fig. 1: (a) Self-consistent Poisson–Schrödinger solution for a single module of a THz QCL using a tight-binding boundary conditions. (b) Lowest conduction and highest valence band states computed using an empirical pseudopotential model for a periodic array of Ge quantum dots in a Si host crystal. (c) Impurity scattering rates as a function of subband separation in infinite quantum wells of varying width.

New functionality includes efficient numerical solvers for the Schrodinger/Poisson equations, enabling self-consistent computation of the bandstructure in generic 1D potentials [e.g., Fig. 1(a)], impurity and excitonic states and annealed systems. Bandstructure in quantum wires and dots can be found using quasi-analytical models or empirical pseudopotential calculations [Fig. 1(b)]. New carrier-scattering functionality is provided, including interactions with impurities [Fig. 1(c)], acoustic/LO phonons, interface roughness, alloy disorder and carrier–carrier processes. A one-dimensional thermal model enables the temperature profile to be computed for arbitrary multi-layered structures, in response to pulsed or continuous power sources.

Infrastructure has been put in place for community-driven development, coordinated through a project on the Launchpad website [3]. A three-tiered hierarchical software architecture has been developed, allowing considerable flexibility in its usage, including an Application Programmers Interface (API) in C++, a set of ready-made "building-block" programs for running elemental, common modelling tasks and a set of example UNIX scripts suitable for non-expert users.

[1] Nextnano, http://www.nextnano.de
[2] Quantum wells, wires and dots (QWWAD), http://launchpad.net/qwwad
[3] P. Harrison and A. Valavanis, Quantum Wells, Wires and Dots, 4th Ed. Wiley, Chichester (2015).