Project title:
Theory of the optoelectronic properties of inter-band cascade light-emitting diodes

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Project description:

There is increasing interest in the development of compact and inexpensive semiconductor light sources operating at mid-infrared wavelengths due to their potential for a wide variety of sensing applications, including monitoring of atomospheric pollutants, chemical process control, and detection of biological markers in non-invasive medical diagnostics, in addition to potential applications in free-space optical communications. For example, due to the presence of strong absorption features in the vibrational-rotational spectra of the important greenhouse gases methane (CH_4) and carbon dioxide (CO_2) at respective wavelengths of 3.3 and 4.2 μm, devices operating at these wavelengths are of particular interest for environmental monitoring.

In the past decade, so-called inter- and intra-band cascade devices have become well established at wavelengths > 3 μm. However, these are complicated multi-quantum well structures requiring careful design and optimisation: a typical cascade active region consists of up to 100 layers, with tight tolerances on layer thickness and material composition.

The focus of this project will be to establish accurate simulations of the electronic band structure and optical emission spectra for real inter-band cascade structures, with a view to developing an understanding of their properties from the perspective of applications in mid-infrared inter-band cascade light-emitting diodes (IC-LEDs). The aim in the first instance will be to establish calculations for real IC-LED structures, the results of which can be compared to data provided by experimental collaborators in order to elucidate the origins of the observed properties of existing prototype IC-LEDs.

To achieve this the student will firstly establish calculations of the single-particle eigenstates in real IC-LED structures, based on a numerical solution of the (multi-band) Schrödinger equation for arbitrary multi-quantum well structures. The student will then use these single particle eigenstates as input to compute the radiative recombination rate in IC-LED structures. Time permitting, a theoretical survey will be undertaken in order to (i) identify general trends in the properties and performance of IC-LEDs and, on this basis, (ii) identify candidate optimised structures offering high performance.

Additional information:

The project will be theoretical/computational in nature. This project is suitable for students who have taken at least two of PY2105 (Introduction to Computational Physics), PY3102 (Quantum Mechanics), or PY3105 (Introduction to Condensed Matter Physics), and who have some basic familiarity with a programming/scripting language (e.g. C/C++, Python or MATLAB). The student will develop practical experience working in a Linux computing environment, in the development of scientific software, and in numerical simulation of photonic devices. Aspects of the project work will be similar in nature to that encountered in module PY4109 (Advanced Computational Physics), and would hence be advantageous to a student enrolled in this module.