Master / Semester Thesis

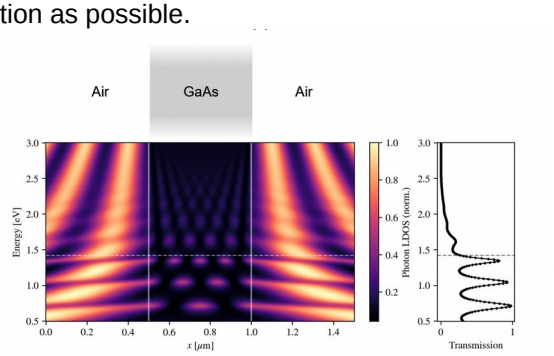
Quantum-Kinetic Simulations of Light-Matter Interactions

The Big Picture

Understanding light-matter interactions at the nanoscale is indispensable for the development of future optoelectronic devices, be it more efficient nanostructured photovoltaic cells, on-chip-photodiodes, or nano-LEDs. Due to their nanoscale footprint, accurate simulation of such devices requires one to capture all the quantum mechanical processes at play. To this end, quantum-kinetic simulations based on the non-equilibrium Green's function (NEGF) formalism are a powerful and versatile tool. A unified quantum-kinetic simulation framework, capturing light and matter at this level of theory can deliver device design guidelines that greatly reduce the development cost and allow a look at the cross-section of physics at play.

Project Description

Our quantum transport simulator is currently being extended to also include the effects of microscopic electron-photon scattering. We compute the optical degrees of freedom on a finite-element mesh and couple them to the electronic states, represented in a localized orbital basis. Unfortunately, even under approximation, the computation of the photon-electron scattering terms can take up a significant portion of the simulation time. We thus employ specialized numerical techniques and rely on HPC techniques to make as much use of paralellization/hardware acceleration as possible.



Localized density of photon states for a slab of GaAs in air.

Type of Work

The type of work can be adjusted to your interests:

- First principles electronic structure calculations of 2D material heterostructures
- Theoretical investigation (developing computational models and/or analysis of algorithms)
- Hands-on code development

Prerequisites

We are looking for candidates with a strong interest in physics, computational materials science and software development. Fundamental knowledge of quantum mechanics and solid state physics are required. Programming skills in Python / C++ are highly desirable. Naturally, experience with quantum transport and density functional theory are advantageous.

Status: Available

Looking for 1 Semester/Master student
Interested candidates please contact: Nicolas Vetsch vetschn@iis.ee.ethz.ch
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