

Summer Research Project (Undergraduate Placement)

Title

Post-processing and Experimental Interpretation of Second-Harmonic Generation Spectra from First-Principles Simulations

Project Overview

Second-Harmonic Generation (SHG) is a nonlinear optical process widely used to probe symmetry, electronic structure, and dimensionality in materials. It is especially powerful for two-dimensional and layered systems, where confinement and broken inversion symmetry can lead to strong SHG signals.

First-principles simulation codes such as LUMEN/YAMBO can compute the microscopic nonlinear optical response of materials, providing access to SHG spectra. However, the simulation output (e.g. second-order susceptibilities) cannot be directly compared with experimental measurements. Additional post-processing and optical modelling are required to obtain the SH intensity measured in experiments.

This project aims to bridge this gap by developing a Python-based post-processing workflow that connects first-principles SHG simulations with experimentally relevant observables.

Project Description

You will develop and implement a Python post-processing code to extract SHG data from LUMEN/YAMBO simulations and compute the corresponding second-harmonic intensity using established theoretical models. The implementation will be integrated into Yambopy, the Python framework used for analyzing YAMBO/LUMEN calculations.

The project provides hands-on experience at the interface of computational materials science, nonlinear optics, and scientific programming.

For more information contact the project supervisor: Dr Myrta Gruening (m.gruening@qub.ac.uk)

Background and Skills

The project is suitable for advanced undergraduate students in physics, applied mathematics, or related fields.

Required: basic Python programming skills and interest in condensed matter or optical spectroscopy or scientific programming.

Not required: prior knowledge of/experience with nonlinear optics, first-principles methods and the YAMBO/LUMEN/Yambopy codes.

Duration and Support

- Duration: 8 weeks/20 hours per week
- Stipend: 2,000 GBP