Lumabi: a Python package to streamline the computation of phonon-resolved luminescence spectra of defects and dopants in solids

07 August 2025

Summary

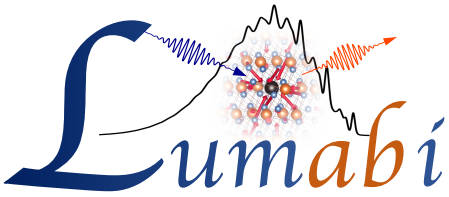

Figure 1: Lumabi logo

Lumabi is a Python package within the AbiPy framework (Gonze et al. 2020) that automates the computation of phonon-resolved luminescence spectra of point defects and dopants in inorganic solids using the ABINIT first-principles software (Gonze et al. 2020). The package provides an end-to-end workflow: from ΔSCF density-functional theory calculations with constrained occupations, to the generation of defect phonon modes in large supercells, right through the generation of luminescence spectra based on Huang–Rhys theory (Huang and Rhys 1950; Jin et al. 2021).

Lumabi addresses the growing need for reproducible, automated workflows in defect physics (Lejaeghere et al. 2016; Bosoni et al. 2024), with applications ranging from quantum technologies (Wolfowicz et al. 2021; Dreyer et al. 2018) to phosphors for solid-state lighting (Pust, Schmidt, and Schnick 2015; Lin, Karlsson, and Bettinelli 2017; Fang et al. 2022). Tutorials and examples are available in the AbiPy Book.

Statement of need

Defect-induced luminescence plays a key role in materials design for optoelectronics, quantum information, and phosphor technologies. Accurate predictions require ground- and excited-state calculations, phonon computations, and multiple post-processing steps, which are typically laborious to set up.

Existing tools focus either on defect energetics (Naik and Jain 2018; Péan et al. 2017; Goyal et al. 2017; Broberg et al. 2018; Kumagai et al. 2021; Neilson and Murphy 2022; Arrigoni and Madsen 2021; Shen and Varley 2024) or luminescence post-processing (Kavanagh et al. 2024; Turiansky et al. 2021; Cavignac, Jobic, and Latouche 2024), and most are tied to the commercial VASP software (Kresse and Furthmüller 1996). To our knowledge, no open-source package has provided a fully automated pipeline for computing defect phonon modes in large supercells together with luminescence spectra.

Lumabi aims at filling this gap. Built on ABINIT and AbiPy, with interfaces to Phonopy (Togo and Tanaka 2015; Togo 2023) and Pymatgen (Ong et al. 2013), it streamlines the entire workflow. It enables reproducible simulations with limited intervention and produces structured data suitable for data-driven searches (Hariyani et al. 2023) and machine learning (Lee et al. 2025).

Software Description, Features, and Computational Workflow

The code is organized into four modules that can be combined into a complete workflow or used independently. We describe here the overall working principles of each module. For a more practical approach, we provide online tutorials.

LumiWork Module

A computational workflow for calculating phonon-resolved photoluminescence (PL) spectra of defect systems starts with the LumiWork module, which automates ABINIT DFT tasks with ΔSCF constrained occupations (Jones and Gunnarsson 1989; Hellman, Razaznejad, and Lundqvist 2004). Users provide the defect supercell structure, the DFT input parameters, and constrained occupations of the Kohn-Sham states designed to mimic the excited state of the system under study. This module manages two structural relaxations for the ground- and the excited-state, and offers optional static SCF computations followed by non-SCF band structure calculations. As the relaxed excited state is not known in advance, input files are generated dynamically.

ΔSCF Post-Processing Module

The next step in the workflow is handled by the ΔSCF post-processing module. This tool takes the NetCDF output files generated by the previous Lu-

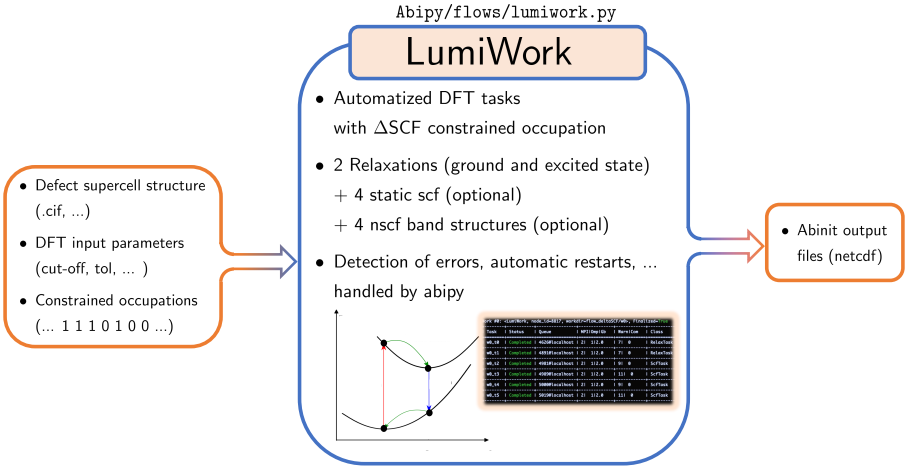

Figure 2: The LumiWork module, an AbiPy Workflow that automates ABINIT DFT tasks with ΔSCF constrained occupations.

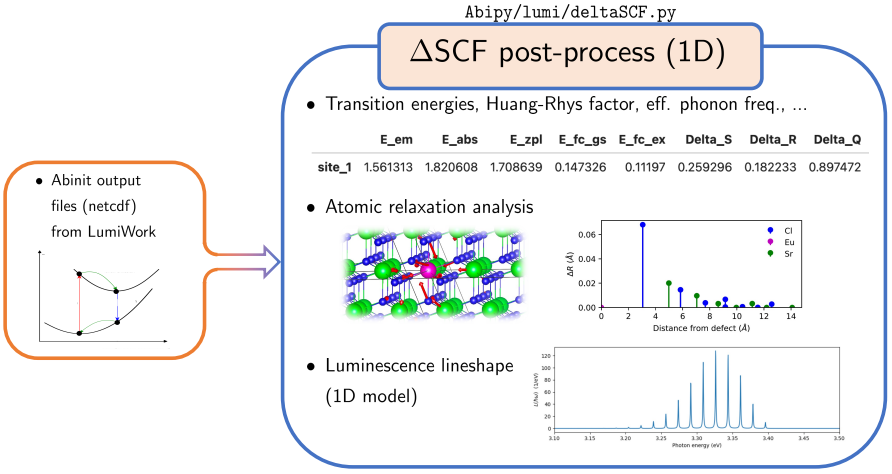

Figure 3: The ΔSCF module, designed to post-process ΔSCF constrained-occupation calculations using a one-dimensional configuration-coordinate model.

miWork module, and processes them following a one-dimensional configuration-coordinate model (Jia et al. 2017; Bouquiaux et al. 2021). This analysis provides insights into the luminescence characteristics of the defect under study by computing properties such as transition energies, Huang-Rhys factors, effective phonon frequencies, and lineshapes following this 1D model or within a semi-classical approximation. It also facilitates the analysis of atomic relaxations by, for example, automatically generating VESTA (Momma and Izumi 2011) files that include relaxation vectors.

IFCs Embedding Module

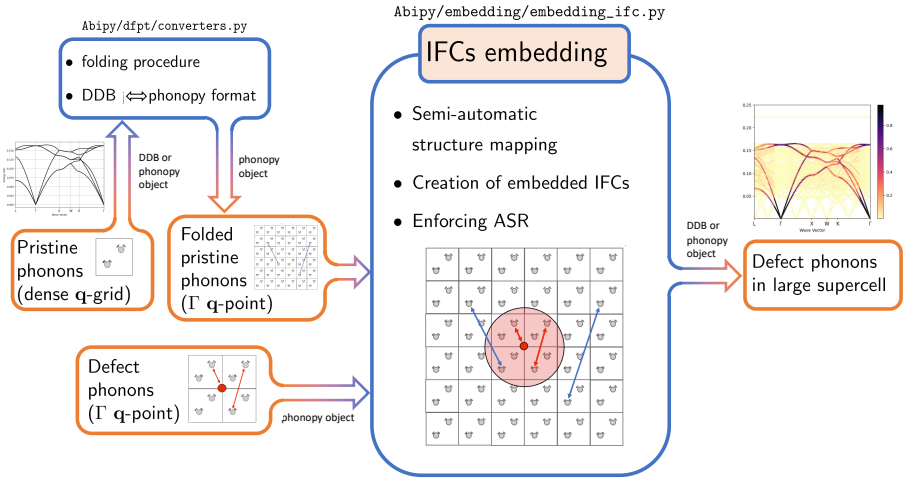

Figure 4: The IFCs embedding module, allowing to calculate defect phonons in large supercells.

The Interatomic Force Constants (IFCs) Embedding module enables defect phonon calculations in large supercells, which are otherwise computationally prohibitive with standard density-functional perturbation theory or finite differences approach. The method combines short-range defect force constants, obtained in a small supercell, with pristine host force constants computed from the bulk and folded into a large supercell. The resulting embedded IFC matrix captures both localized defect modes and host phonons, allowing accurate spectral simulations at dilute defect concentrations. The implementation interfaces with Phonopy and produces phonon objects compatible with later analysis. First employed in the context of the luminescence of the NV center by Alkauskas et al. (Alkauskas et al. 2014), this embedding approach has been then used in various materials (Jin et al. 2021; Bouquiaux et al. 2023; Razinkovas et al. 2021; Maciaszek et al. 2023; Jin, Govoni, and Galli 2022). For the mathematical details and the technical implementation, we refer to the accompanying

Jupyter Book.

Lineshape Calculation Module

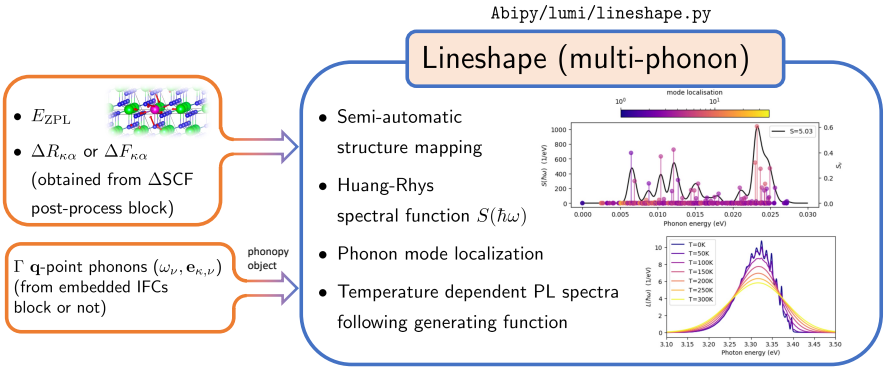

Figure 5: The lineshape module, allowing to compute the temperature-dependent spectra.

As a final step, the Lineshape module is used. The main task of this module is to compute the Huang-Rhys spectral function $S(\hbar\omega)$ (Alkauskas et al. 2014; Bouquiaux et al. 2023) and to generate temperature-dependent PL spectra using the efficient generating function approach (Jin et al. 2021).

The code takes as input the zero-phonon line energy, the atomic displacements $\Delta R_{\kappa\alpha}$ or forces $\Delta F_{\kappa\alpha}$ induced by the electronic transition (obtained from the ΔSCF post-processing step), and the phonon modes provided as a Phonopy object (potentially obtained from the IFCs embedding module). Notice that the use of the displacements is only compatible if the phonon supercell is of the same size as the ΔSCF supercell. The use of the forces (equivalent under the harmonic approximation) allows one to use efficiently the previous block and enlarge the supercell size, ensuring a good convergence of the Huang-Rhys spectral function (Alkauskas et al. 2014; Jin et al. 2021; Bouquiaux et al. 2023). An analysis of the different phonon mode localization can also be performed.

Examples and Applications

This computational workflow has been used for inorganic phosphors activated with Eu^{2+} dopants and has also been tested on a variety of other systems including F-centers (oxygen vacancy) in CaO and the NV center in diamond.

Its versatility allows for any kind of point defect. These developments have been particularly useful in understanding the luminescence properties of technologically significant red-emitting Eu-doped phosphor materials. Notably, the workflow has been applied to $SrAl_2Li_2O_2N_2$:Eu^{2+} and $SrLiAl_3N_4$:Eu^{2+}, shedding new light on their phonon sideband (Bouquiaux et al. 2021, 2023). We refer the reader to the accompanying notebook tutorials for practical examples demonstrating the application of this workflow.

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