




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

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DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

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Submitted: 17 July 2025

Published: unpublished

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Summary

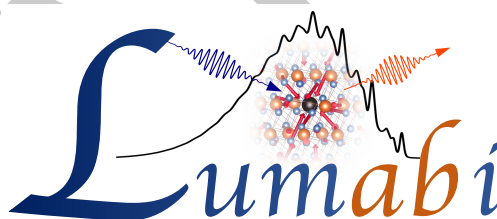


Figure 1: Lumabi logo

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 Δ SCF 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 & Rhys, 1950; Jin et al., 2021).

Lumabi addresses the growing need for reproducible, automated workflows in defect physics (Bosoni et al., 2024; Lejaeghere et al., 2016), with applications ranging from quantum technologies (Dreyer et al., 2018; Wolfowicz et al., 2021) to phosphors for solid-state lighting (Fang et al., 2022; Lin et al., 2017; Pust et al., 2015). 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 (Arrigoni & Madsen, 2021; Broberg et al., 2018; Goyal et al., 2017; Kumagai et al., 2021; Naik & Jain, 2018; Neilson & Murphy, 2022; Péan et al., 2017; Shen & Varley, 2024) or luminescence post-processing (Cavignac et al., 2024; Kavanagh et al., 2024; Turiansky et al., 2021), and most are tied to the commercial VASP software (Kresse & 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, 2023; Togo & Tanaka, 2015) 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

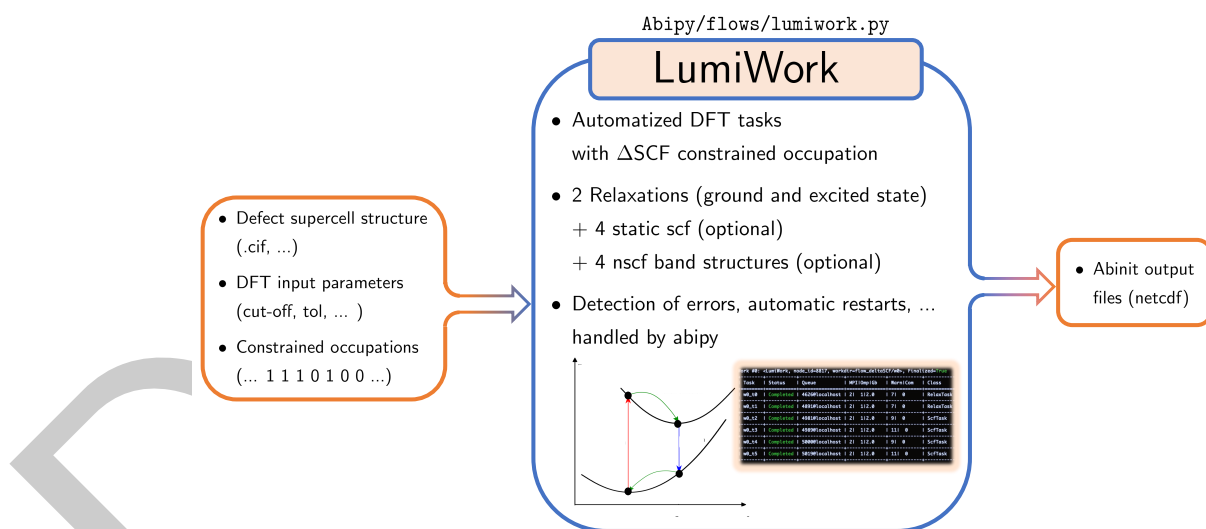


Figure 2: The LumiWork module, an AbiPy Workflow that automates ABINIT DFT tasks with Δ SCF constrained occupations.

A computational workflow for calculating phonon-resolved photoluminescence (PL) spectra of defect systems starts with the LumiWork module, which automates ABINIT DFT tasks with Δ SCF constrained occupations (Hellman et al., 2004; Jones & Gunnarsson, 1989). 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.

55 Δ SCF Post-Processing Module

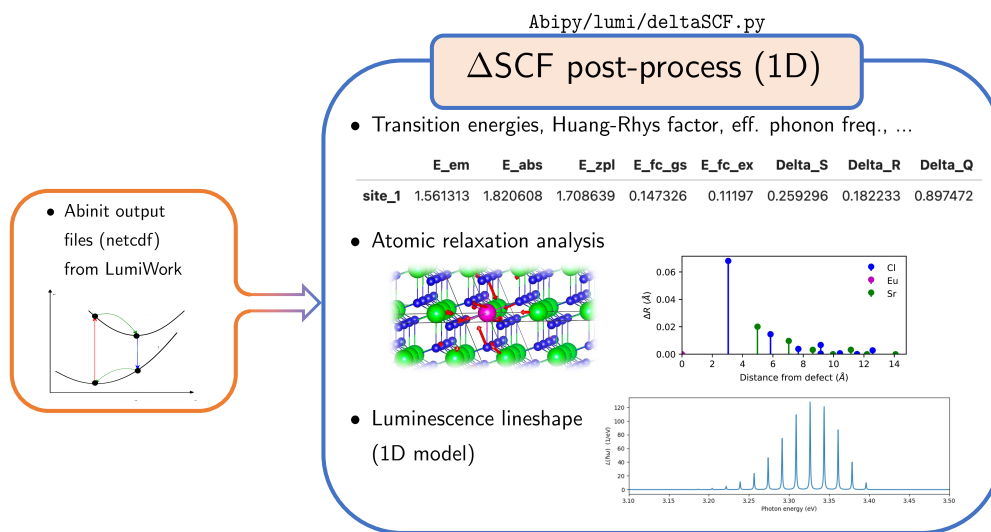


Figure 3: The Δ SCF module, designed to post-process Δ SCF constrained-occupation calculations using a one-dimensional configuration-coordinate model.

56 The next step in the workflow is handled by the Δ SCF post-processing module. This tool takes
 57 the NetCDF output files generated by the previous LumiWork module, and processes them
 58 following a one-dimensional configuration-coordinate model (Bouquiaux et al., 2021; Jia et al.,
 59 2017). This analysis provides insights into the luminescence characteristics of the defect under
 60 study by computing properties such as transition energies, Huang-Rhys factors, effective phonon
 61 frequencies, and lineshapes following this 1D model or within a semi-classical approximation.
 62 It also facilitates the analysis of atomic relaxations by, for example, automatically generating
 63 VESTA (Momma & Izumi, 2011) files that include relaxation vectors.

64 IFCs Embedding Module

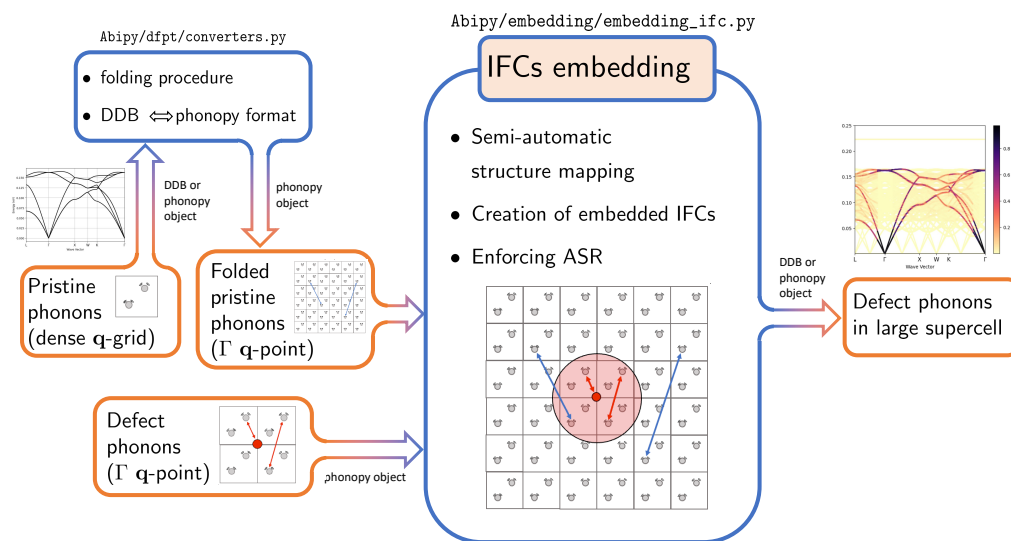


Figure 4: The IFCs embedding module, allowing to calculate defect phonons in large supercells.

65 The Interatomic Force Constants (IFCs) Embedding module enables defect phonon calculations
 66 in large supercells, which are otherwise computationally prohibitive with standard density-
 67 functional perturbation theory or finite differences approach. The method combines short-range
 68 defect force constants, obtained in a small supercell, with pristine host force constants computed
 69 from the bulk and folded into a large supercell. The resulting embedded IFC matrix captures
 70 both localized defect modes and host phonons, allowing accurate spectral simulations at dilute
 71 defect concentrations. The implementation interfaces with Phonopy and produces phonon
 72 objects compatible with later analysis. First employed in the context of the luminescence of
 73 the NV center by Alkauskas et al. (Alkauskas et al., 2014), this embedding approach has been
 74 then used in various materials (Bouquiaux et al., 2023; Jin et al., 2021, 2022; Maciaszek et al.,
 75 2023; Razinkovas et al., 2021). For the mathematical details and the technical implementation,
 76 we refer to the accompanying [Jupyter Book](#).

77 Lineshape Calculation Module

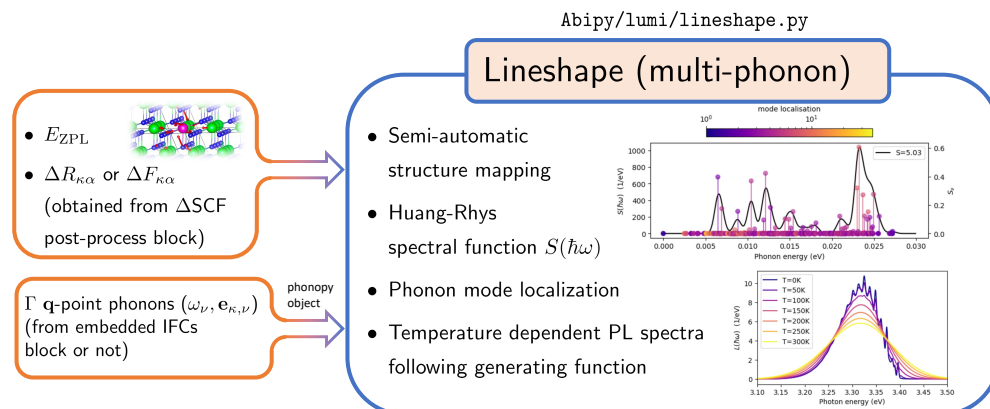


Figure 5: The lineshape module, allowing to compute the temperature-dependent spectra.

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

82 The code takes as input the zero-phonon line energy, the atomic displacements $\Delta R_{\kappa\alpha}$ or forces
83 $\Delta F_{\kappa\alpha}$ induced by the electronic transition (obtained from the Δ SCF post-processing step),
84 and the phonon modes provided as a Phonopy object (potentially obtained from the IFCs
85 embedding module). Notice that the use of the displacements is only compatible if the phonon
86 supercell is of the same size as the Δ SCF supercell. The use of the forces (equivalent under
87 the harmonic approximation) allows one to use efficiently the previous block and enlarge the
88 supercell size, ensuring a good convergence of the Huang-Rhys spectral function (Alkauskas et
89 al., 2014; Bouquiaux et al., 2023; Jin et al., 2021). An analysis of the different phonon mode
90 localization can also be performed.

91 Examples and Applications

92 This computational workflow has been used for inorganic phosphors activated with Eu^{2+}
93 dopants and has also been tested on a variety of other systems including F-centers (oxygen
94 vacancy) in CaO and the NV center in diamond. Its versatility allows for any kind of point
95 defect. These developments have been particularly useful in understanding the luminescence
96 properties of technologically significant red-emitting Eu-doped phosphor materials. Notably,
97 the workflow has been applied to $\text{SrAl}_2\text{Li}_2\text{O}_2\text{N}_2:\text{Eu}^{2+}$ and $\text{SrLiAl}_3\text{N}_4:\text{Eu}^{2+}$, shedding new
98 light on their phonon sideband (Bouquiaux et al., 2021, 2023). We refer the reader to the
99 accompanying notebook tutorials for practical examples demonstrating the application of this
100 workflow.

Acknowledgements

J.B. acknowledge support from the F.R.S.-FNRS. S.P. is a Research Associate of the Fonds de la Recherche Scientifique - FNRS. X.G. also acknowledges support from the F.R.S.-FNRS, under grant n°T.0103.19 (PDR - ALPS). S.P. also acknowledges support from the Walloon Region in the strategic axe FRFS-WEL-T. This work was supported by the Communauté française de Belgique through the SURFASCOPE project (ARC 19/24-102). Y.J acknowledges the funding support from National Key R&D Program (No.2022YFB3503800), Natural Science Foundation of Hebei Province (No.E2021203126) and Cultivation Project for Basic Research and Innovation of Yanshan University (No.2021LGQN033). Computational resources have been provided by the Consortium des Équipements de Calcul Intensif (CÉCI), funded by the FRS-FNRS under Grant No. 2.5020.11 and by the Walloon Region.

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