Summary

Lumabi logo

Lumabi is a Python package ~~integrated~~ within the AbiPy framework [@gonze2020abinit] ~~designed to automate and streamline~~that automates the computation of phonon-resolved luminescence spectra of point defects ~~(including the case of dopants)~~and dopants in inorganic solids using the ABINIT first-principles software ~~application~~ [~~@gonze2002first;@gonze2009abinit;@gonze2016recent;~~@gonze2020abinit]. The package ~~addresses the growing need for efficient, reproducible workflows in materials science [@lejaeghere2~~ an end-to-end workflow: from ~~quantum technologies [@wolfowicz2021quantum;@dreyer2018first] to down-conve~~ ΔSCF density-functional theory calculations with constrained occupations, to the generation of defect phonon modes in large supercells, right through the ~~final~~ generation of luminescence spectra based on ~~the Huang-~~Huang–Rhys theory [@huang1950theory;@jin2021photoluminescence].~~ A collection of tutorials~~

Lumabi addresses the growing need for reproducible, automated workflows in defect physics [@lejaeghere2016reproducibility;@bosoni2024verify], with applications ranging from quantum technologies [@wolfowicz2021quantum;@dreyer2018first] to phosphors for solid-state lighting [@pust2015revolution;@lin2017inorganic;@fang2022evolutionary]. Tutorials and ~~examples, organized as Jupyter Books, is~~examples are available ~~on~~in the AbiPy Book.

Statement of need

~~The study of defect-~~Defect-induced luminescence plays a key role in materials ~~is crucial~~design for ~~understanding~~optoelectronics, quantum information, and ~~designing materials with specific optical properties. However, the computational workflow required to accurat~~ technologies. Accurate predictions require ground- and excited-state calculations, phonon computations, ~~as well as pre-~~ andmultiple post-processing ~~steps.~~steps, which are typically laborious to set up.

~~Therefore, a number of software packages have been developed to manage the pre- or post-processing of~~Existi tools focus either on defect ~~calculations~~energetics [@naik2018coffee;@pean2017presentation;@goyal2017computatio or luminescence post-processing [@Kavanagh2024;@turiansky2021nonrad;@cavignac2024], and most are ~~all interfaced with~~tied to the commercial VASP software~~ VASP~~ [@kresse1996efficiency]~~, and only provide the post-processing part of DFT computations following the formalis~~ To our knowledge, ~~the generation of~~no open-source package has provided a fully automated pipeline for computing defect phonon modes in large supercells ~~following an embedding of the interatomic force constants is currently not available.~~together with luminescence spectra.

~~Divided in four main Python modules,~~ Lumabi ~~provides a solution~~aims at filling this gap. Built on ABINIT and AbiPy, with interfaces to ~~automate all the necessary tasks required to compute phonon-resolved luminescence spectra of defects. The d~~ [~~@gonze2002first;@gonze2009abinit;@gonze2016recent;@gonze2020abinit]~~@togo2015first;@togo2023first]~~. The g~~ and~~ post-processing are done with the AbiPy package, which is interfaced with~~

Pymatgen [@ong2013python]~~. Lumabi is also interfaced with~~, it streamlines the ~~Phonopy package [@togo2015first;@togo2023first] for the calculations of phonons. This tool is intended for res~~ workflow. It enables reproducible simulations with ~~minimal human intervention. Moreover, the systematic gener~~ intervention and produces structured data ~~through this automated workflow could enable~~suitable for data-driven searches ~~for new phosphors~~ [@hariyani2023guide] and ~~could provide a robust foundation for training machine-~~machine learning ~~models~~ [@lee2025machine] ~~to accelerate the discovery of materials with targeted luminescent properties.~~.

Software Description, Features, and Computational Workflow

The code is ~~structured around~~organized into four ~~Python modules, each handling a different stage of the compu~~ ~~are designed to work seamlessly together—where the output of one serves as the input to the next—each indiv~~ can be ~~also~~combined into a complete workflow or used ~~independently with ease. In this article, we~~independently. We describe here the overall working principles of each ~~block.~~module. For a more practical approach, we provide ~~online tutorials for the different modules.~~online tutorials.

LumiWork Module

The LumiWork module, an AbiPy Workflow that automates ABINIT DFT tasks with ΔSCF 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 ΔSCF constrained occupations [@jones1989density;@hellman2004potential]. Users provide the defect supercell ~~structure (e.g. in CIF format),~~structure, the DFT input ~~parameters (e.g., the plane-wave kinetic energy cutoff, the stopping SCF criterion, etc.),~~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. ~~Note that the workflow is dynamic: since~~As the relaxed excited state is not known ~~beforehand,~~in advance, input files ~~must be~~are generated ~~at run-time.~~

~~The `LumiWork` class inherits from the Abipy's `Work` class. Consequently, it leverages error detection and autom~~

dynamically.

ΔSCF Post-Processing Module

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

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 Lumi-

Work module, and processes them following a one-dimensional configuration-coordinate model [@jia2017first;@bouquiaux2021importance]. This analysis provides ~~detailed~~ 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 [@momma2011vesta] files that include relaxation vectors.

~~In cases where experimental lineshapes exhibit resolved phonon peaks, it is important to note that the linesha~~

IFCs Embedding Module

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

The Interatomic Force Constants (IFCs) Embedding module ~~computes the~~enables defect phonon ~~of defected materials~~calculations in large ~~supercells~~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 ~~the $\mathbf{q} = (0, 0, 0)$\(\) (Γ\(\) point) wave vector. This module addresses the computational challenges associate~~
defect concentrations. The implementation interfaces with ~~capturing both the coupling~~Phonopy
and produces phonon objects compatible with ~~long-wavelength phonons and the localized phonon modes introdu~~
analysis. First employed in the context of the luminescence of the NV center by Alkauskas et al. [@alkauskas2014], ~~the~~this embedding approach has been then used in various materials [@jin2021photoluminescence;@bouquiaux2023first;@razinkovas2021vibrational;@maciasz
~~The procedure relies on~~For the ~~short-range nature of interatomic forces to build IFCs matrices for defect supe~~
details and the ~~dilute limit.~~

~~First, the real-space IFCs for the defect system $C^{\text{defect}}_{\kappa\alpha,\kappa'\alpha'}$\(\) are computed within a relatively small supercell.~~

~~Second, the IFCs of the pristine system $C^{\text{pristine}}_{\kappa\alpha,\kappa'\alpha'}$\(\) are computed in a much larger supercell. A practical app~~

~~Third, an embedded IFC matrix $C^{\text{emb}}_{\kappa\alpha,\kappa'\alpha'}$\(\) is constructed using the following rules: if both atoms κ\(\) and~~
implementation, we refer to the ~~pristine value: $C^{\text{emb}}_{\kappa\alpha,\kappa'\alpha'} = C^{\text{pristine}}_{\kappa\alpha,\kappa'\alpha'}$\(\)~~accompanying
Jupyter Book. ~~The cut-off radius R_c\(\) is typically determined by the size of the initial supercell used to com~~

~~The code performs a mapping between the structures of the pristine and defect computations. Such mapping~~

Lineshape Calculation Module

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 $S(\hbar\omega)$ [@alkauskas2014;

@bouquiaux2023first] and to generate temperature-dependent PL spectra using the efficient generating function approach [@jin2021photoluminescence].

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 [@alkauskas2014;@jin2021photoluminescence;@bouquiaux2023first]. 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 [@bouquiaux2021importance;@bouquiaux2023first]. We refer the reader to the accompanying notebook tutorials for practical examples demonstrating the application of this workflow.

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References