LumiSpy Release 0.2

The LumiSpy developers

Apr 29, 2022

USER GUIDE

1 Contents	3
Bibliography	33
Python Module Index	35
Index	37

LumiSpy is a Python package extending the functionality for multi-dimensional data analysis provided by the HyperSpy library. It is aimed at helping with the analysis of luminescence spectroscopy data (cathodoluminescence, photoluminescence, electroluminescence, Raman, SNOM).

Check out the Installation section for further information, including how to start using this project.

Complementing this documentation, the LumiSpy Demos repository contains curated Jupyter notebooks to provide tutorials and exemplary workflows.

Note: This project is under active development. Everyone is welcome to contribute. Please read our (see *Contributing*) guidelines and get started!

CHAPTER

ONE

CONTENTS

1.1 Installation

Follow these 3 steps to install LumiSpy.

1.1.1 Creating a conda environment

LumiSpy requires Python 3 and conda - we suggest using the Python 3 version of Miniconda.

We recommend creating a new environment for the LumiSpy package (or installing it in the HyperSpy environment, if you have one already). To create a new environment:

- 1. Load the anaconda prompt.
- 2. Run the following command:

```
(base) conda create -n lumispy
```

1.1.2 Installing the package in the new environment

Now activate the LumiSpy environment and install the package using pip:

(base) conda activate lumispy (lumispy) pip install lumispy

Installation is completed! To start using it, check the next section.

1.1.3 Getting Started

To get started using LumiSpy, especially if you are unfamiliar with Python, we recommend using Jupyter notebooks. Having installed LumiSpy as above, a Jupyter notebook can be opened using the following commands entered into an anaconda prompt (from scratch):

```
(base) conda activate lumispy
(lumispy) jupyter lab
```

1.2 Introduction

1.2.1 What is LumiSpy

LumiSpy is an open-source python library aimed at helping with the analysis of luminescence spectroscopy data – the development started mainly with photoluminescence (PL), cathodoluminescence (CL), electroluminescence (EL) and Raman spectroscopy in mind. Besides the standard continuous-excitation spectral data, the idea is to provide tools also for the analysis of time-resolved (transient) measurements. However, it may prove useful also for other optical measurements, such as absorption or transmission spectroscopy, scanning optical near field miscroscopy (SNOM), as well as fourier-transform infrared spectroscopy (FTIR).

LumiSpy is an extension to the python package `HyperSpy <https://hyperspy.org>`_ that facilitates hyperspectral data analysis, i.e. maps or linescans where a spectrum is collected at each pixel. Or more general, multidimensional datasets that can be described as multidimensional arrays of a given signal. Notable features that HyperSpy provides are:

- base signal classes for the handling of (multidimensional) spectral data,
- the necessary tools for loading various data file formats with a focus on electron microscopy
- analytical tools that exploit the multidimensionality of datasets,
- a user-friendly and powerful framework for model fitting that provides many standard functions and can be easily extended to custom ones,
- machine learning algorithms that can be useful e.g. for denoising data,
- efficient handling of big datasets,,
- functions for data visualization both to evaluate datasets during the analysis and provide interactive operation for certain functions, as well as for plotting of data.
- extracting subsets of data from multidimensional datasets via regions of interest and a powerful numpy-style indexing mechanism,
- handling of non-uniform data axes (introduced in the v1.7 release).

LumiSpy provides in particular:

- additional Signal types specifically for luminescence spectra and transients,
- transformation to signal_axis for use of other units, such as electron Volt and wavenumbers (Raman shift),
- various utility functions useful in luminescence spectroscopy data analysis, such as joining multiple spectra along the signal axis, normalizing data, etc.

LumiSpy should facilitate an easy and reproducible analysis of single spectra or spectral images

1.2.2 Signal types

As an extension to HyperSpy, LumiSpy provides several signal types extending the base classes available in HyperSpy. When the LumiSpy library is installed, these additional signal types are directly available to HyperSpy. To print all available specialised hyperspy.signal.BaseSignal subclasses installed in your system call the hyperspy.utils. print_known_signal_types() function:

>>> hs.print_known_signal_types()

The different subclasses are characterized by the signal_type metadata attribute. Some additional properties are summarized in the table below. Depending on the use case, certain functions will only be available for some signal types (or inheriting) signal types.

BaseSignal	sig-	sig-	dtype	aliases
subclass	nal_dimensio	n nal_type		
LumiSpectrum	1	Lumines-	real	LuminescenceSpectrum
		cence		
CLSpectrum	1	CL	real	CLSpectrum, cathodoluminescence
CLSEMSpectrum	1	CL_SEM	real	CLSEM, cathodoluminescence SEM
CLSTEMSpectrum	1 1	CL_STEM	real	CLSTEM, cathodoluminescence STEM
ELSpectrum	1	EL	real	ELSpectrum, electroluminescence
PLSpectrum	1	PL	real	PLSpectrum, photoluminescence
LumiTransient	1	Transient	real	TRLumi, TR luminescence, time-resolved luminescence
LumiTransient	2	Tran-	real	TRLumiSpec, TR luminescence spectrum, time-resolved
		sientSpec		luminescence spectrum

Table	1:	LumiSpy	subclasses	and	their	basic	attributes.
rabic	1.	Lumopy	subclasses	ana	unen	ousie	autioutes.

The hierarchy of the LumiSpy signal types and their inheritance from HyperSpy is summarized in the following diagram:

```
└── hyperspy.signal.BaseSignal
```

hyperspy._signals.signal1d.Signal1D
 LumiSpectrum
 || CLSpectrum
 || CLSEMSpectrum
 || CLSTEMSpectrum
 || ELSpectrum
 LumiTransient
 LumiTransient
 LumiTransientSpectrum

1.2.3 Where are we heading?

LumiSpy is under active development, and as a user-driven project, we welcome contributions (see *Contributing*) to the code and documentation from any other users.

Currently, we have implemented the base functionality that extends HyperSpy's capabilities to additional signal classes. In the near future, the following functions should be developed:

- handling of transient (time-resolved) data,
- reading of common PL data formats,
- more dedicated analysis functionalities,
- ...

1.3 Non-uniform signal axes

LumiSpy facilitates the use of non-uniform axes, where the points of the axis vector are not uniformly spaced. This situation occurs in particular when converting a wavelength scale to energy (eV) or wavenumbers (e.g. for Raman shifts).

The conversion of the signal axis can be performed using the functions $to_eV()$, $to_invcm()$ and $to_raman_shift()$ (alias for $to_invcm_relative()$). If the unit of the signal axis is set, the functions can handle wavelengths in either nm or μ m.

Accepted parameters are inplace=True/False (default is True), which determines whether the current signal object is modified or a new one is created, and jacobian=True/False (default is True, see *Jacobian transformation*).

1.3.1 The energy axis

The transformation from wavelength λ to energy E is defined as $E = hc/\lambda$. Taking into account the permittivity of air and doing a conversion from nm to eV, we get:

$$E = \frac{10^9 hc}{e\epsilon_r \lambda},$$

where h is the Planck constant, c is the speed of light, e is the elementary charge and ϵ_r is the relative permittivity of air.

>>> s2 = s.to_eV(inplace=False)
>>> s.to_eV()

Note: The relative permittivity of air ϵ_r is wavelength dependent. This dependence is taken into account by LumiSpy based on the analytical formula given by [Peck] valid from 185-1700 nm (outside of this range, the permittivity values at the edges of the range are used and a warning is raised).

1.3.2 The wavenumber axis/Raman shifts

The transformation from wavelength λ to wavenumber $\tilde{\nu}$ (spatial frequency of the wave) is defined as $\tilde{\nu} = 1/\lambda$. The wavenumber is usually given in units of cm⁻¹.

When converting a signal to Raman shift, i.e. the shift in wavenumbers from the exciting laser wavelength, the laser wavelength has to be passed to the function using the parameter laser using the same units as for the original axis (e.g. 325 for nm or 0.325 for μ m) unless it is contained in the *LumiSpy metadata structure* under Acquisition_instrument.Laser.wavelength.

TODO: Automatically read laser wavelength from metadata if given there.

```
>>> s2 = s.to_invcm(inplace=False)
>>> s.to_invcm()
>>> s2 = s.to_raman_shift(inplace=False, laser=325)
>>> s.to_raman_shift(laser=325)
```

1.3.3 Jacobian transformation

When transforming the signal axis, the signal intensity is automatically rescaled (Jacobian transformation), unless the jacobian=False option is given. Only converting the signal axis, and leaving the signal intensity unchanged, implies that the integral of the signal over the same interval would lead to different results depending on the quantity on the axis (see e.g. [Mooney].).

For the energy axis as example, if we require $I(E)dE = I(\lambda)d\lambda$, then $E = hc/\lambda$ implies

$$I(E) = I(\lambda) \frac{d\lambda}{dE} = I(\lambda) \frac{d}{dE} \frac{hc}{\lambda} = -I(\lambda) \frac{hc}{E^2}$$

The minus sign just reflects the different directions of integration in the wavelength and energy domains. The same argument holds for the conversion from wavelength to wavenumber (just without the additional prefactors in the equation). The renormalization in LumiSpy is defined such that the intensity is converted from counts/nm (or counts/ μ m) to counts/meV. The following figure illustrates the effect of the Jacobian transformation:



Transformation of the variance

Scaling the signal intensities implies that also the stored variance of the signal needs to be scaled accordingly. According to $Var(aX) = a^2 Var(X)$, the variance has to be multiplied with the square of the Jacobian. This squared renormalization is automatically performed by LumiSpy if jacobian=True. In particular, homoscedastic (constant) noise will consequently become heteroscedastic (changing as a function of the signal axis vector). Therefore, if the metadata.Signal.Noise_properties.variance attribute is a constant, it is converted into a hyperspy.signal. BaseSignal object before the transformation.

See *Signal variance (noise)* for more general information on data variance in the context of model fitting and the HyperSpy documentation on setting the noise properties.

Note: If the Jacobian transformation is performed, the values of metadata.Signal.Noise_properties. Variance_linear_model are reset to their default values (gain_factor=1, gain_offset=0 and correlation_factor=1). Should these values deviate from the defaults, make sure to run hyperspy.signal. BaseSignal.estimate_poissonian_noise_variance() prior to the transformation.

References

1.4 Fitting luminescence data

LumiSpy is compatible with HyperSpy model fitting. It can fit using both uniform and and non-uniform axes (e.g. energy scale). A general introduction can be found in the HyperSpy user guide.

TODO: Note on advantages of fitting signals in the eV axis (not restricted to Gaussians). See e.g. [Wang]

TODO: Show how to extract the modeled signal with all/one component.

See also the LumiSpy demo notebooks for examples of data fitting.

1.4.1 Signal variance (noise)

TODO: Documentation on variance handling in the context of fitting, in particular using hyperspy.signal. BaseSignal.estimate_poissonian_noise_variance()

References

1.5 LumiSpy metadata structure

LumiSpy extends the HyperSpy metadata structure with conventions for metadata specific to its signal types. Refer to the HyperSpy metadata documentation for general metadata fields.

The metadata of any **signal objects** is stored in the *metadata* attribute, which has a tree structure. By convention, the node labels are capitalized and the ones for leaves are not capitalized. When a leaf contains a quantity that is not dimensionless, the units can be given in an extra leaf with the same label followed by the _units suffix.

Besides directly accesing the metadata tree structure, e.g. s.metadata.Signal.signal_type, the Hyper-Spy methods hyperspy.misc.utils.DictionaryTreeBrowser.set_item(), hyperspy.misc.utils. DictionaryTreeBrowser.has_item() and hyperspy.misc.utils.DictionaryTreeBrowser.get_item() can be used to add to, search for and read from items in the metadata tree, respectively.

The luminescence specific metadata structure is represented in the following tree diagram. The default units are given in parentheses. Details about the leaves can be found in the following sections of this chapter. Note that not all types of leaves will apply to every type of measurement. For example, while parallel acquisition with a CCD is characterized by the central_wavelength, a serial acquisition with a PMT will require a start_wavelength and a step_size.

(continues on next page)

(continued from previous page)

<pre>objective_magnification Filter filter_type position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) # for SEM/TEM see HyperSpy Spectrometer model acquisition_mode entrance_slit_width (nm) exit_slit_width (nm) exit_slit_width (nm) start_wavelength (nm) start_wavelength (nm) start_start_wavelength (nm) Grating Grating Grating Grating Grating Grating Grating Gratina_angle (°) blazing_angle (°) blazing_mavelength (nm) Filter filter_type position optical_density cut_on_wavelength (nm) Detector Grating Grat</pre>		— power (mW)
<pre>Filter filter_type position optical_density cut_on_wavelength (nm) for SEM/TEM see HyperSpy Spectrometer model acquisition_mode entrance_slit_width (nm) central_wavelength (nm) start_wavelength (nm) start_wavelength (nm) step_size (nm) Grating groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter filter_type position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— objective_magnification
<pre>filter_type</pre>		— Filter
<pre>position</pre>		— filter_type
<pre>optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) # for SEM/TEM see HyperSpy Spectrometer model acquisition_mode entrance_slit_width (mm) central_wavelength (nm) start_wavelength (nm) step_size (nm) Grating groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter filter_type position optical_density cut_on_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm)</pre>		— position
<pre>cut_on_wavelength (nm) cut_off_wavelength (nm) # for SEM/TEM see HyperSpy Spectrometer model acquisition_mode entrance_slit_width (mm) central_wavelength (nm) start_wavelength (nm) start_wavelength (nm) step_size (nm) Grating Grating Grating Grating Filter filter_type position optical_density cut_on_wavelength (nm) Cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— optical_density
<pre>cut_off_wavelength (nm) # for SEM/TEM see HyperSpy Spectrometer model acquisition_mode entrance_slit_width (mm) exit_slit_width (mm) central_wavelength (nm) start_wavelength (nm) start_wavelength (nm) step_size (nm) Grating groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter filter_type position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		<pre> cut_on_wavelength (nm)</pre>
<pre># for SEM/TEM see HyperSpy Spectrometer model acquisition_mode entrance_slit_width (mm) central_wavelength (nm) start_wavelength (nm) start_wavelength (nm) Grating Grating Grating Grating Filter Filter Filter Filter Filter Optical_density Cut_on_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		<pre> cut_off_wavelength (nm)</pre>
<pre>Spectrometer model acquisition_mode entrance_slit_width (mm) exit_slit_width (mm) central_wavelength (nm) start_wavelength (nm) start_wavelength (nm) Grating groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter filter_type position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>	L	— # for SEM/TEM see HyperSpy
<pre>model acquisition_mode entrance_slit_width (mm) central_wavelength (nm) start_wavelength (nm) start_wavelength (nm) groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter filter_type position optical_density cut_off_wavelength (nm) cut_off_wavelength (nm) frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>	— s	pectrometer
<pre>acquisition_mode entrance_slit_width (mm) central_wavelength (nm) start_wavelength (nm) start_wavelength (nm) step_size (nm) Grating groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter filter_type position optical_density cut_off_wavelength (nm) cut_off_wavelength (nm) detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— model
<pre>entrance_slit_width (mm) exit_slit_width (mm) central_wavelength (nm) start_wavelength (nm) step_size (nm) Grating groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter i filter_type position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— acquisition_mode
<pre>exit_slit_width (mm) central_wavelength (nm) start_wavelength (nm) step_size (nm) Grating groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter i filter_type position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		<pre>— entrance_slit_width (mm)</pre>
<pre>central_wavelength (nm) start_wavelength (nm) Grating Grating Grating Grating Blazing_angle (°) Blazing_wavelength (nm) Filter Filter Filter Filter Optical_density Cut_on_wavelength (nm) Cut_off_wavelength (nm) Detector Getector Getector_type model Frames integration_time (s) saturation_fraction binning processing sensor_roi jixel_size (µm) Spectral_image</pre>		— exit_slit_width (mm)
<pre>start_wavelength (nm) step_size (nm) Grating groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter filter_type position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi jixel_size (µm) Spectral_image</pre>		— central_wavelength (nm)
<pre>step_size (nm) Grating Grating Grating Grating Grating Grating Blazing_angle (°) Blazing_wavelength (nm) Filter Filter Filter Optical_density Cut_on_wavelength (nm) Cut_off_wavelength (nm) Detector Getector Getector_type Model Frames Integration_time (s) Saturation_fraction Dinning Processing Sensor_roi Jixel_size (µm) Spectral_image</pre>		— start_wavelength (nm)
Grating Gra		— step_size (nm)
<pre>groove_density (grooves/mm) blazing_angle (°) blazing_wavelength (nm) Filter position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		- Grating
<pre>blazing_angle (°) blazing_wavelength (nm) Filter position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) betector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		<pre> groove_density (grooves/mm)</pre>
<pre>blazing_wavelength (nm) Filter position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi jixel_size (µm) Spectral_image</pre>		— blazing_angle (°)
<pre>Filter Filter Filt</pre>		└── blazing_wavelength (nm)
<pre>filter_type position optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>	L	— Filter
<pre>position</pre>		— filter_type
<pre>optical_density cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		- position
<pre>cut_on_wavelength (nm) cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		<pre> optical_density</pre>
<pre>cut_off_wavelength (nm) Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		<pre> cut_on_wavelength (nm)</pre>
<pre>Detector detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		<pre> cut_off_wavelength (nm)</pre>
<pre>detector_type model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>	— D	etector
<pre>model frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— detector_type
<pre>frames integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— model
<pre>integration_time (s) saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— frames
<pre>saturation_fraction binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— integration_time (s)
<pre>binning processing sensor_roi pixel_size (µm) Spectral_image</pre>		— saturation_fraction
<pre>processing sensor_roi pixel_size (µm) Spectral_image</pre>		— binning
<pre> sensor_roi pixel_size (µm) Spectral_image</pre>		— processing
└── pixel_size (µm) └── Spectral_image		— sensor_roi
Spectral_image		— pixel_size (µm)
	L S	pectral_image
— mode	ŀ	— mode
— drift_correction_periodicity	ŀ	— drift_correction_periodicity
<pre>drift_correction_units (s)</pre>	L	<pre>— drift_correction_units (s)</pre>

1.5.1 General

See HyperSpy-Metadata-General.

1.5.2 Sample

See HyperSpy-Metadata-Sample.

1.5.3 Signal

signal_type type: string

String that describes the type of signal. The LumiSpy specific signal classes are summarized under Signal types.

quantity type: string

The name of the quantity of the "intensity axis" with the units in round brackets if required, for example 'Intensity (counts/s)'.

See HyperSpy-Metadata-Signal for additional fields.

1.5.4 Acquisition Instrument

1.5.5 Laser / SEM / TEM

For SEM or TEM see HyperSpy-Metadata-SEM or HyperSpy-Metadata-TEM.

Laser

laser_type type: string

The type of laser used, e.g. 'HeCd'.

model type: string

Model of the laser (branding by manufacturer).

wavelength type: float

Emission wavelength of the exciting laser in nm.

power type: float

Measured power of the excitation laser in mW.

magnification type: int

Magnification of the microscope objective used to focus the beam to the sample.

Filter

Information about additional filters entered into the lightpath before the sample. In case multiple filters are used, they should be numbered *Filter_1*, etc.

filter_type type: string

Type of filter (e.g. 'optical density', 'short pass', 'long pass', 'bandpass', 'color').

position type: string

Position in the beam (e.g. 'excitation' vs. 'detection' in case of optical excitation).

optical_density type: float

Optical density in case of an intensity filter.

cut_on_wavelength type: float

Cut on wavelength in nm in case of a long-pass or bandpass filter.

cut_off_wavelength type: float

Cut off wavelength in nm in case of a short-pass or bandpass filter.

1.5.6 Spectrometer

Contains information about the spectrometer, configuration and grating used for the measurement. In case multiple spectrometers are connected in series, they should be numbered *Spectrometer_1*, etc.

model type: string

Model of the spectrometer (branding by manufacturer).

acquisition_mode type: string

Acquisition mode (e.g. 'Parallel dispersive', versus 'Serial dispersive').

entrance_slit_width type: float

Width of the entrance slit in mm.

exit_slit_width type: float

Width of the exit slit (serial acquisition) in mm.

central_wavelength type: float

Central wavelength during acquisition (parallel acquisition).

start_wavelength type: float

Start wavelength in nm (serial acquisition).

step_size type: float

Step size in nm (serial acquisition).

Grating

Information of the dispersion grating employed in the measurement.

groove_density type: int

Density of lines on the grating in grooves/mm.

blazing_angle type: int

Angle in degree (^o) that the grating is blazed at.

blazing_wavelength type: int

Wavelength that the grating blaze is optimized for in nm.

Filter

Information about additional filters entered into the lightpath after the sample. In case multiple filters are used, they should be numbered *Filter_1*, etc. See filter-label above for details on items that may potentially be included.

1.5.7 Detector

Contains information about the detector used to acquire the signal. Contained leaves will differ depending on the type of detector.

detector_type type: string

The type of detector used to acquire the signal (CCD, PMT, StreakCamera, TCSPD).

model type: string

The model of the used detector.

frames type: int

Number of frames that are summed to yield the total integration time.

integration_time (s) type: float

Time over which the signal is integrated. In case multiple frames are summed, it is the total exposure time. In case of serial acquisition, it is the dwell time per data point.

saturation_fraction type: float

Fraction of the signal intensity compared with the saturation threshold of the CCD.

binning type: tuple of int

A tuple that describes the binning of a parallel detector such a CCD on readout in x and y directions.

processing type: string

Information about automatic processing performed on the data, e.g. 'dark subtracted'.

sensor_roi type: tuple of int

Tuple of length 2 or 4 that specifies range of pixels on a detector that are read out: (offset x, offset y, size x, size y) for a 2D array detector and (offset, size) for a 1D line detector.

pixel_size type: float or tuple of float

Size of a pixel in µm. Tuple of length 2 (width, height), when the pixel is not square.

1.5.8 Spectral_image

Contains information about mapping parameters, such as step size, drift correction, etc.

mode type: string

Mode of the spectrum image acquisition such as 'Map' or 'Linescan'.

drift_correction_periodicity type: int/float

Periodicity of the drift correction in specified units (standard s).

drift_correction_units type: string

Units of the drift correction such as 's', 'px', 'rows'.

1.6 lumispy

1.6.1 lumispy package

Subpackages

lumispy.signals package

Submodules

lumispy.signals.cl_spectrum module

Signal class for cathodoluminescence spectral data

class lumispy.signals.cl_spectrum.CLSEMSpectrum(*args, **kwargs)

Bases: lumispy.signals.cl_spectrum.CLSpectrum

1D scanning electron microscopy cathodoluminescence signal class.

correct_grating_shift(*cal_factor_x_axis*, *corr_factor_grating*, *sem_magnification*, **kwargs)

Applies shift caused by the grating offset wrt the scanning centre. Authorship: Gunnar Kusch (gk419@cam.ac.uk)

Parameters

- cal_factor_x_axis The navigation correction factor.
- **corr_factor_grating** The grating correction factor.
- **sem_magnification** The SEM (real) magnification value. For the Attolight original metadata, take the *SEM.Real_Magnification* value
- **kwargs** The parameters passed to *hyperspy.align1D()* function like: interpolation_method ('linear', 'nearest', 'zero', 'slinear', 'quadratic, 'cubic') parallel: Bool crop, expand, fill_value ...

class lumispy.signals.cl_spectrum.CLSTEMSpectrum(*args, **kwargs)

Bases: lumispy.signals.cl_spectrum.CLSpectrum

1D scanning transmission electron microscopy cathodoluminescence signal class.

class lumispy.signals.cl_spectrum.CLSpectrum(*args, **kwargs)

Bases: lumispy.signals.luminescence_spectrum.LumiSpectrum

General 1D cathodoluminescence signal class.

_make_signal_mask(luminescence_roi)

Creates a mask from the peak position and peak widths of the luminescence spectrum.

Parameters luminescence_roi (*array*) – In the form of an array of pairwise elements [[peak1_x, peak1_width], [peak2_x, peak2_width],...].

Returns A *signal_mask*.

Return type array

remove_spikes(*threshold='auto'*, *show_diagnosis_histogram=False*, *inplace=False*,

*luminescence_roi=None, signal_mask=None, add_noise=False, navigation_mask=None, interactive=False, **kwargs)*

HyperSpy-based spike removal tool adapted to LumiSpy to run non-interactively and without noise addition by default. Graphical interface to remove spikes from EELS spectra or luminescence data. If noninteractive, it removes all spikes and returns a *~hyperspy.signals_signal_tools.SpikesRemoval* object.

Parameters

- **signal_mask** (*bool array*) Restricts the operation to the signal locations not marked as True (masked).
- **navigation_mask** (*bool array*) Restricts the operation to the navigation locations not marked as True (masked).
- **threshold** (*'auto'* or *int*) if *int* set the threshold value use for the detecting the spikes. If *auto*, determine the threshold value as being the first zero value in the histogram obtained from the spikes_diagnosis() method.
- **interactive** (*bool*) If True, remove the spikes using the graphical user interface. If False, remove all the spikes automatically, which can introduce artefacts if used with signal containing peak-like features. However, this can be mitigated by using the *signal_mask* argument to mask the signal of interest.
- **display** (*bool*) If True, display the user interface widgets. If False, return the widgets container in a dictionary, usually for customisation or testing.
- **toolkit** (*str*, *iterable of strings or None*) If None (default), all available widgets are displayed or returned. If string, only the widgets of the selected toolkit are displayed if available. If an interable of toolkit strings, the widgets of all listed toolkits are displayed or returned.
- ****kwargs** (*dict*) -

Keyword arguments pass to SpikesRemoval()

See also:

spikes_diagnosis()

- show_diagnosis_histogram (bool) Plot or not the derivative histogram to show the magnitude of the spikes present.
- **inplace** (*bool*) If False, a new signal object is created and returned. If True, the original signal object is modified.

• **luminescence_roi** (*array*) – The peak position and peak widths of the peaks in the luminescence spectrum. In the form of an array of pairwise elements [[peak1_x, peak1_width], [peak2_x, peak2_width],...] in the units of the signal axis. It creates a signal_mask protecting the peak regions. To be used instead of *signal_mask*.

Returns Depends on inplace, returns or overwrites the CLSpectrum after spike removal.

Return type None or CLSpectrum

class lumispy.signals.cl_spectrum.LazyCLSEMSpectrum(*args, **kwargs)

Bases: hyperspy._signals.lazy.LazySignal, lumispy.signals.cl_spectrum.CLSEMSpectrum

Lazy 1D scanning electron microscopy cathodoluminescence signal class.

class lumispy.signals.cl_spectrum.LazyCLSTEMSpectrum(*args, **kwargs)

Bases: hyperspy._signals.lazy.LazySignal, lumispy.signals.cl_spectrum.CLSTEMSpectrum

Lazy 1D scanning transmission electron microscopy cathodoluminescence signal class.

class lumispy.signals.cl_spectrum.LazyCLSpectrum(*args, **kwargs)

Bases: hyperspy._signals.lazy.LazySignal, lumispy.signals.cl_spectrum.CLSpectrum

General lazy 1D cathodoluminescence signal class.

lumispy.signals.common_luminescence module

Signal class for luminescence data (BaseSignal class)

class lumispy.signals.common_luminescence.CommonLumi

Bases: object

General luminescence signal class (dimensionless)

crop_edges(crop_px)

Crop the amount of pixels from the four edges of the scanning region, from out the edges inwards.

Parameters crop_px (*int*) – Amount of pixels to be cropped on each side individually.

Returns signal_cropped – A smaller cropped CL signal object. If inplace is True, the original object is modified and no LumiSpectrum is returned.

Return type CommonLuminescence

normalize(*pos=nan*, *element_wise=False*, *inplace=False*)

Normalizes data to value at pos along signal axis, defaults to maximum value.

Can be helpful for e.g. plotting, but does not make sense to use on signals that will be used as input for further calculations!

- **pos** (*float*, *int*) If 'nan' (default), spectra are normalized to the maximum. If *float*, position along signal axis in calibrated units at which to normalize the spectra. If *int*, index along signal axis at which to normalize the spectra.
- **element_wise** (*boolean*) If *False* (default), a spectrum image is normalized by a common factor. If *True*, each spectrum is normalized individually.
- **inplace** (*boolean*) If *False* (default), a new signal object is created and returned. If *True*, the operation is performed on the existing signal object.

Notes

Sets *metadata.Signal.normalized* to *True*. If *metadata.Signal.quantity* contains the word 'Intensity', replaces this field with 'Normalized intensity'.

remove_negative(basevalue=1, inplace=True)

Sets all negative values to 'basevalue', e.g. for logarithmic scale plots.

Parameters

- **basevalue** (*float*) Value by which negative values are replaced (default = 1).
- **inplace** (*boolean*) If *False*, a new signal object is created and returned. Otherwise (default) the operation is performed on the existing signal object.

Notes

Sets metadata.Signal.negative_removed to True.

scale_by_exposure(integration_time=None, inplace=False, **kwargs)

Scale data in spectrum by integration time / exposure, (e.g. convert counts to counts/s).

Parameters

- **integration_time** (*float*) Integration time (exposure) in s. If not given, the function tries to use the 'metadata.Acquisition_instrument.Detector.integration_time' field or alternatively find any 'integration_time', 'exposure' or 'dwell_time' fields in the *original_metadata*.
- **inplace** (*boolean*) If *False* (default), a new signal object is created and returned. If *True*, the operation is performed on the existing signal object.

Notes

Sets metadata.Signal.scaled to True. If intensity units is 'counts', replaces them by 'counts/s'.

Deprecated since version 0.2: The *exposure* argument was renamed *integration_time*, and it will be removed in LumiSpy 1.0.

lumispy.signals.common_transient module

Signal class for transient data (BaseSignal class)

class lumispy.signals.common_transient.CommonTransient

Bases: object

General transient signal class (dimensionless)

lumispy.signals.el_spectrum module

Signal class for electroluminescence spectral data

class lumispy.signals.el_spectrum.ELSpectrum(*args, **kwargs)
Bases: lumispy.signals.luminescence_spectrum.LumiSpectrum

General 1D electroluminescence signal class

class lumispy.signals.el_spectrum.LazyELSpectrum(*args, **kwargs)
Bases: hyperspy._signals.lazy.LazySignal, lumispy.signals.el_spectrum.ELSpectrum

General lazy 1D electroluminescence signal class

lumispy.signals.luminescence_spectrum module

Signal class for Luminescence spectral data (1D).

class lumispy.signals.luminescence_spectrum.LazyLumiSpectrum(*args, **kwargs)

Bases: hyperspy._signals.lazy.LazySignal, lumispy.signals.luminescence_spectrum. LumiSpectrum

General lazy 1D luminescence signal class.

class lumispy.signals.luminescence_spectrum.LumiSpectrum(*args, **kwargs)

Bases: hyperspy._signals.signal1d.Signal1D, lumispy.signals.common_luminescence. CommonLumi

General 1D luminescence signal class.

_reset_variance_linear_model()

Resets the variance linear model parameters to their default values, as they are not applicable any longer after a Jacobian transformation.

px_to_nm_grating_solver(gamma_deg, deviation_angle_deg, focal_length_mm, ccd_width_mm, grating_central_wavelength_nm, grating_density_gr_mm, inplace=False)

Converts signal axis of 1D signal (in pixels) to wavelength, solving the grating equation. See *lu-mispy.axes.solve_grating_equation* for more details.

- **gamma_deg** (*float*) Inclination angle between the focal plane and the centre of the grating (found experimentally from calibration). In degree.
- deviation_angle_deg (float) Also known as included angle. It is defined as the difference between angle of diffraction (β) and angle of incidence (α). Given by manufacturer specsheet. In degree.
- **focal_length_mm** (*float*) Given by manufacturer specsheet. In mm.
- ccd_width_mm (float) The width of the CDD. Given by manufacturer specsheet. In mm.
- grating_central_wavelength_nm (float) Wavelength at the centre of the grating, where exit slit is placed. In nm.
- grating_density_gr_mm (int) Grating density in gratings per mm.

• **inplace** (*bool*) – If False, it returns a new object with the transformation. If True, the original object is transformed, returning no object.

Returns signal – A signal with calibrated wavelength units.

Return type LumiSpectrum

Examples

```
>>> s = LumiSpectrum(np.ones(20),))
>>> s.px_to_nm_grating_solver(*params, inplace=True)
>>> s.axes_manager.signal_axes[0].units == 'nm'
```

remove_background_from_file(background=None, inplace=False, **kwargs)

Subtract the background to the signal in all navigation axes. If no background file is passed as argument, the *remove_background()* from HyperSpy is called with the GUI.

Parameters

- **background** (*array shape (2, n) or Signal1D*) An array containing the background x-axis and the intensity values [[xs],[ys]] or a Signal1D object. If the x-axis values do not match the signal_axes, then interpolation is done before subtraction. If only the intensity values are provided, [ys], the functions assumes no interpolation needed.
- **inplace** (*boolean*) If False, it returns a new object with the transformation. If True, the original object is transformed, returning no object.

Returns signal – A background subtracted signal.

Return type LumiSpectrum

Notes

This function does not work with non-uniform axes.

savetxt(filename, fmt='%.5f', delimiter=\t', axes=True, transpose=False, **kwargs)

Writes luminescence spectrum object to simple text file.

Writes single spectra to a two-column data file with signal axis as X and data as Y. Writes linescan data to file with signal axis as first row and navigation axis as first column (flipped if *transpose=True*).

- filename (string) -
- fmt (*str or sequence of strs, optional*) A single or sequence of format strings. Default is '%.5f'.
- **delimiter** (*str*, *optional*) String or character separating columns. Default is ','
- **axes** (*bool*, *optional*) If True (default), include axes in saved file. If False, save the data array only.
- **transpose** (*bool*, *optional*) If True, transpose data array and exchange axes. Default is false. Ignored for single spectra.
- ****kwargs** Takes any additional arguments of numpy.loadtxt, e.g. *newline header*, *footer*, *comments*, or *encoding*.

See also:

numpy.savetxt

Examples

```
>>> import lumispy as lum
>>> import numpy as np
. . .
>>> # Spectrum:
>>> S = lum.signals.LumiSpectrum(np.arange(5))
>>> S.savetxt('spectrum.txt')
            0.00000
0.00000
1.00000
            1.00000
2.00000
            2.00000
3.00000
            3.00000
4.00000
            4.00000
. . .
>>> # Linescan:
>>> L = lum.signals.LumiSpectrum(np.arange(25).reshape((5,5)))
>>> L.savetxt('linescan.txt')
0.00000
           0.00000 1.00000 2.00000 3.00000 4.00000
0.00000
                                                             20.00000
            0.00000 5.00000 10.00000
                                            15.00000
1.00000
           1.00000 6.00000 11.00000
                                             16.00000
                                                             21.00000
2.00000
           2.00000 7.00000 12.00000
                                             17.00000
                                                             22.00000
3.00000
           3.00000 8.00000 13.00000
                                             18.00000
                                                             23.00000
4.00000
            4.00000 9.00000 14.00000
                                             19.00000
                                                             24.00000
```

to_array(axes=True, transpose=False)

Returns luminescence spectrum object as numpy array (optionally including the axes).

Returns single spectra as two-column array. Returns linescan data as array with signal axis as first row and navigation axis as first column (flipped if *transpose=True*).

- **axes** (*bool*, *optional*) If True (default), include axes in array. If False, return the data array only.
- **transpose** (*bool*, *optional*) If True, transpose data array and exchange axes. Default is false. Ignored for single spectra.
- ****kwargs** Takes any additional arguments of numpy.loadtxt, e.g. *newline header, footer, comments*, or *encoding*.

Notes

The output of this function can be used to convert a signal object to a pandas dataframe, e.g. using $df = pd.Dataframe(S.to_array())$.

Examples

```
>>> import lumispy as lum
>>> import numpy as np
. . .
>>> # Spectrum:
>>> S = lum.signals.LumiSpectrum(np.arange(5))
>>> S.to_array()
array([[0., 0.],
      [1., 1.],
      [2., 2.],
     [3., 3.],
      [4., 4.]])
. . .
>>> # Linescan:
>>> L = lum.signals.LumiSpectrum(np.arange(25).reshape((5,5)))
>>> L.to_array()
array([[ 0., 0., 1., 2., 3., 4.],
     [0., 0., 1., 2., 3., 4.],
      [1., 5., 6., 7., 8., 9.],
      [ 2., 10., 11., 12., 13., 14.],
      [ 3., 15., 16., 17., 18., 19.],
      [ 4., 20., 21., 22., 23., 24.]])
```

to_eV(inplace=True, jacobian=True)

Converts signal axis of 1D signal to non-linear energy axis (eV) using wavelength dependent permittivity of air. Assumes wavelength in units of nm unless the axis units are specifically set to μ m.

The intensity is converted from counts/nm (counts/µm) to counts/meV by doing a Jacobian transformation, see e.g. Mooney and Kambhampati, J. Phys. Chem. Lett. 4, 3316 (2013), doi:10.1021/jz401508t, which ensures that integrated signals are correct also in the energy domain. If the variance of the signal is known, i.e. *metadata.Signal.Noise_properties.variance* is a signal representing the variance, a squared renormalization of the variance is performed. Note that if the variance is a number (not a signal instance), it is converted to a signal if the Jacobian transformation is performed

- **inplace** (*boolean*) If *False*, a new signal object is created and returned. Otherwise (default) the operation is performed on the existing signal object.
- **jacobian** (*boolean*) The default is to do the Jacobian transformation (recommended at least for luminescence signals), but the transformation can be suppressed by setting this option to *False*.

Examples

```
>>> import numpy as np
>>> from lumispy import LumiSpectrum
>>> S1 = LumiSpectrum(np.ones(20), DataAxis(axis = np.arange(200,400,10)), ))
>>> S1.to_eV()
```

to_invcm(inplace=True, jacobian=True)

Converts signal axis of 1D signal to non-linear wavenumber axis (cm⁻¹). Assumes wavelength in units of nm unless the axis units are specifically set to μ m.

The intensity is converted from counts/nm (counts/µm) to counts/cm^-1 by doing a Jacobian transformation, see e.g. Mooney and Kambhampati, J. Phys. Chem. Lett. 4, 3316 (2013), doi:10.1021/jz401508t, which ensures that integrated signals are correct also in the wavenumber domain. If the variance of the signal is known, i.e. *metadata.Signal.Noise_properties.variance* is a signal representing the variance, a squared renormalization of the variance is performed. Note that if the variance is a number (not a signal instance), it is converted to a signal if the Jacobian transformation is performed.

Parameters

- **inplace** (*boolean*) If *False*, a new signal object is created and returned. Otherwise (default) the operation is performed on the existing signal object.
- **jacobian** (*boolean*) The default is to do the Jacobian transformation (recommended at least for luminescence signals), but the transformation can be suppressed by setting this option to *False*.

Examples

```
>>> import numpy as np
>>> from lumispy import LumiSpectrum
>>> S1 = LumiSpectrum(np.ones(20), DataAxis(axis = np.arange(200,400,10)), ))
>>> S1.to_invcm()
```

to_invcm_relative(laser=None, inplace=True, jacobian=True)

Converts signal axis of 1D signal to non-linear wavenumber axis (cm^-1) relative to the exciting laser wavelength (Stokes/Anti-Stokes shift). Assumes wavelength in units of nm unless the axis units are specifically set to µm.

The intensity is converted from counts/nm (counts/µm) to counts/cm^-1 by doing a Jacobian transformation, see e.g. Mooney and Kambhampati, J. Phys. Chem. Lett. 4, 3316 (2013), doi:10.1021/jz401508t, which ensures that integrated signals are correct also in the wavenumber domain. If the variance of the signal is known, i.e. *metadata.Signal.Noise_properties.variance* is a signal representing the variance, a squared renormalization of the variance is performed. Note that if the variance is a number (not a signal instance), it is converted to a signal if the Jacobian transformation is performed.

- **inplace** (*boolean*) If *False*, a new signal object is created and returned. Otherwise (default) the operation is performed on the existing signal object.
- **jacobian** (*boolean*) The default is to do the Jacobian transformation (recommended at least for luminescence signals), but the transformation can be suppressed by setting this option to *False*.
- **laser** (*float or None*) Laser wavelength in the same units as the signal axis. If None (default), checks if it is stored in *metadata.Acquisition_instrument.Laser.wavelength*.

Examples

```
>>> import numpy as np
>>> from lumispy import LumiSpectrum
>>> S1 = LumiSpectrum(np.ones(20), DataAxis(axis = np.arange(200,400,10)), ))
>>> S1.to_invcm(laser=325)
```

to_raman_shift(laser=None, inplace=True, jacobian=True)

Converts signal axis of 1D signal to non-linear wavenumber axis (cm^-1) relative to the exciting laser wavelength (Stokes/Anti-Stokes shift). Assumes wavelength in units of nm unless the axis units are specifically set to µm.

The intensity is converted from counts/nm (counts/µm) to counts/cm⁻¹ by doing a Jacobian transformation, see e.g. Mooney and Kambhampati, J. Phys. Chem. Lett. 4, 3316 (2013), doi:10.1021/jz401508t, which ensures that integrated signals are correct also in the wavenumber domain. If the variance of the signal is known, i.e. *metadata.Signal.Noise_properties.variance* is a signal representing the variance, a squared renormalization of the variance is performed. Note that if the variance is a number (not a signal instance), it is converted to a signal if the Jacobian transformation is performed.

Parameters

- **inplace** (*boolean*) If *False*, a new signal object is created and returned. Otherwise (default) the operation is performed on the existing signal object.
- **jacobian** (*boolean*) The default is to do the Jacobian transformation (recommended at least for luminescence signals), but the transformation can be suppressed by setting this option to *False*.
- **laser** (*float or None*) Laser wavelength in the same units as the signal axis. If None (default), checks if it is stored in *metadata.Acquisition_instrument.Laser.wavelength*.

Examples

```
>>> import numpy as np
>>> from lumispy import LumiSpectrum
>>> S1 = LumiSpectrum(np.ones(20), DataAxis(axis = np.arange(200,400,10)), ))
>>> S1.to_invcm(laser=325)
```

lumispy.signals.luminescence_transient module

Signal class for luminescence transient data (1D)

```
class lumispy.signals.luminescence_transient.LazyLumiTransient(*args, **kwargs)
```

Bases: hyperspy._signals.lazy.LazySignal, lumispy.signals.luminescence_transient. LumiTransient

General lazy 1D luminescence signal class (transient/time resolved)

class lumispy.signals.luminescence_transient.LumiTransient(*args, **kwargs)

Bases: hyperspy._signals.signal1d.Signal1D, lumispy.signals.common_transient. CommonTransient

General 1D luminescence signal class (transient/time resolved)

lumispy.signals.luminescence_transientspec module

Signal class for luminescence transient data (2D)

class lumispy.signals.luminescence_transientspec.LazyLumiTransientSpectrum(*args, **kwargs)
Bases: hyperspy._signals.lazy.LazySignal, lumispy.signals.luminescence_transientspec.
LumiTransientSpectrum

General lazy 2D luminescence signal class (transient/time resolved)

class lumispy.signals.luminescence_transientspec.LumiTransientSpectrum(*args, **kwargs)

Bases: hyperspy__signals.signal2d.Signal2D, lumispy.signals.common_luminescence. CommonLumi, lumispy.signals.common_transient.CommonTransient

General 2D luminescence signal class (transient/time resolved)

lumispy.signals.pl_spectrum module

Signal class for Photoluminescence spectral data

class lumispy.signals.pl_spectrum.LazyPLSpectrum(*args, **kwargs)
Bases: hyperspy._signals.lazy.LazySignal, lumispy.signals.pl_spectrum.PLSpectrum

General lazy 1D photoluminescence signal class

class lumispy.signals.pl_spectrum.PLSpectrum(*args, **kwargs)

Bases: lumispy.signals.luminescence_spectrum.LumiSpectrum

General 1D photoluminescence signal class

Module contents

lumispy.utils package

Submodules

lumispy.utils.axes module

lumispy.utils.axes._n_air(x)

Relative permittivity of air as a function of WL in nm. This analytical function is correct for the range 185-1700 nm. According to *E.R. Peck and K. Reeder. Dispersion of air, J. Opt. Soc. Am.* 62, 958-962 (1972).

lumispy.utils.axes.axis2eV(ax0)

Converts given signal axis to energy scale (eV) using wavelength dependent permittivity of air. Assumes wavelength in units of nm unless the axis units are specifically set to µm.

lumispy.utils.axes.axis2invcm(ax0)

Converts given signal axis to wavenumber scale (cm $^{-1}$). Assumes wavelength in units of nm unless the axis units are specifically set to μ m.

lumispy.utils.axes.data2eV(data, factor, ax0, evaxis)

The intensity is converted from counts/nm (counts/ μ m) to counts/meV by doing a Jacobian transformation, see e.g. Mooney and Kambhampati, J. Phys. Chem. Lett. 4, 3316 (2013). Ensures that integrated signals are still correct.

lumispy.utils.axes.data2invcm(data, factor, invcmaxis)

The intensity is converted from counts/nm (counts/ μ m) to counts/cm $^{-1}$ by doing a Jacobian transformation, see e.g. Mooney and Kambhampati, J. Phys. Chem. Lett. 4, 3316 (2013). Ensures that integrated signals are still correct.

lumispy.utils.axes.eV2nm(x)

Converts energy (eV) to wavelength (nm) using wavelength-dependent permittivity of air.

lumispy.utils.axes.invcm2nm(x)

Converts wavenumber (cm^{-1}) to wavelength (nm).

lumispy.utils.axes.join_spectra(S, r=50, scale=True, average=False, kind='slinear')

Takes list of Signal1D objects and returns a single object with all spectra joined. Joins spectra at the center of the overlapping range. Scales spectra by a factor determined as average over the range *center* -/+ r pixels. Works both for uniform and non-uniform axes (FunctionalDataAxis is converted into a non-uniform DataAxis).

Parameters

- S(list of Signal1D objects (with overlapping signal axes)) -
- **r** (*int*, *optional*) Number of pixels left/right of center (default 50) defining the range over which to determine the scaling factor, has to be less than half of the overlapping pixels. Change the size of r or use *average=True* if the function induces a step in the intensity.
- **scale** (*boolean*, *optional*) If *True* (default), the later spectra in the list are scaled by a factor determined over *center* -/+ *r* pixels. If *False*, spectra are joined without scaling, which will likely induce a step unless *average=True*.
- **average** (*boolean*, *optional*) If *True*, the contribution of the two signals is continuously graded within the range defined by *r* instead of joining at the center of the range (default).
- **kind** (*str*, *optional*) Interpolation method (default 'slinear') to use when joining signals with a uniform signal axes. See *scipy.interpolate.interp1d* for options.

Returns

- A new Signal1D object containing the joined spectra (properties are copied
- from first spectrum).

Examples

```
>>> s1 = hs.signals.Signal1D(np.ones(32))
>>> s2 = hs.signals.Signal1D(np.ones(32)*2)
>>> s2.axes_manager.signal_axes[0].offset = 25
>>> lum.join_spectra([s1,s2],r=2)
<Signal1D, title: , dimensions: (|57)>
```

lumispy.utils.axes.nm2eV(x)

Converts wavelength (nm) to energy (eV) using wavelength-dependent permittivity of air.

lumispy.utils.axes.nm2invcm(x)

Converts wavelength (nm) to wavenumber (cm^{-1}).

Solves the grating equation. See *horiba.com/uk/scientific/products/optics-tutorial/wavelength-pixel-position* for equations.

Parameters

- axis (hyperspy.axis) Axis in pixel units (no units) to convert to wavelength.
- gamma_deg (float) Inclination angle between the focal plane and the centre of the grating (found experimentally from calibration). In degree.
- deviation_angle_deg (float) Also known as included angle. It is defined as the difference between angle of diffraction (β) and angle of incidence (α). Given by manufacturer specsheet. In degree.
- focal_length_mm (float) Given by manufacturer specsheet. In mm.
- ccd_width_mm (float) The width of the CDD. Given by manufacturer specsheet. In mm.
- grating_central_wavelength_nm (float) Wavelength at the centre of the grating, where exit slit is placed. In nm.
- grating_density_gr_mm (int) Grating density in gratings per mm.

Returns axis – HyperSpy axis object.

Return type hyperspy.axis

lumispy.utils.axes.var2eV(variance, factor, ax0, evaxis)

The variance is converted doing a squared Jacobian renormalization to match with the transformation of the data.

lumispy.utils.axes.var2invcm(variance, factor, invcmaxis)

The variance is converted doing a squared Jacobian renormalization to match with the transformation of the data.

lumispy.utils.io module

lumispy.utils.io.savetxt(S, filename, fmt='%.5f', delimiter=\t', axes=True, transpose=False, **kwargs)

Writes signal object to simple text file.

Writes single spectra to a two-column data file with signal axis as X and data as Y. Writes linescan data to file with signal axis as first row and navigation axis as first column (flipped if *transpose=True*). Writes image to file with the navigation axes as first column and first row. Writes 2D data (e.g. map of a fit parameter value) to file with the signal axes as first column and first row.

- filename (string) -
- fmt (*str or sequence of strs, optional*) A single or sequence of format strings. Default is '%.5f'.
- delimiter (str, optional) String or character separating columns. Default is ','
- **axes** (bool, optional) If True (default), include axes in saved file. If False, save the data array only.

- **transpose** (*bool*, *optional*) If True, transpose data array and exchange axes. Default is false. Ignored for single spectra.
- ****kwargs** Takes any additional arguments of numpy.loadtxt, e.g. *newline header*, *footer*, *comments*, or *encoding*.

See also:

numpy.savetxt

Examples

```
>>> import lumispy as lum
>>> import numpy as np
. . .
>>> # Spectrum:
>>> S = lum.signals.LumiSpectrum(np.arange(5))
>>> lum.savetxt(S, 'spectrum.txt')
            0.00000
0.00000
1.00000
            1.00000
2.00000
            2.00000
3.00000
            3.00000
4.00000
            4.00000
. . .
>>> # Linescan:
>>> L = lum.signals.LumiSpectrum(np.arange(25).reshape((5,5)))
>>> lum.savetxt(L, 'linescan.txt')
0.00000
            0.00000 1.00000 2.00000 3.00000 4.00000
0.00000
            0.00000 5.00000 10.00000
                                             15.00000
                                                              20.00000
1.00000
            1.00000 6.00000 11.00000
                                             16.00000
                                                              21.00000
2.00000
            2.00000 7.00000 12.00000
                                             17.00000
                                                              22.00000
3.00000
            3.00000 8.00000 13.00000
                                              18.00000
                                                              23.00000
4.00000
            4.00000 9.00000 14.00000
                                              19.00000
                                                              24.00000
```

lumispy.utils.io.to_array(S, axes=True, transpose=False)

Returns signal object as numpy array (optionally including the axes).

Returns single spectra as two-column array. Returns linescan data as array with signal axis as first row and navigation axis as first column (flipped if *transpose=True*). Returns image as array with the navigation axes as first column and first row. Returns 2D data (e.g. map of a fit parameter value) as array with the signal axes as first column and first row.

- **axes** (*bool*, *optional*) If True (default), include axes in array. If False, return the data array only.
- **transpose** (*bool*, *optional*) If True, transpose data array and exchange axes. Default is false. Ignored for single spectra.
- ****kwargs** Takes any additional arguments of numpy.loadtxt, e.g. *newline header, footer, comments*, or *encoding*.

Notes

The output of this function can be used to convert a signal object to a pandas dataframe, e.g. using $df = pd.Dataframe(lum.to_array(S))$.

Examples

```
>>> import lumispy as lum
>>> import numpy as np
. . .
>>> # Spectrum:
>>> S = lum.signals.LumiSpectrum(np.arange(5))
>>> lum.to_array(S)
array([[0., 0.],
      [1., 1.],
      [2., 2.],
      [3., 3.],
      [4., 4.]])
. . .
>>> # Linescan:
>>> L = lum.signals.LumiSpectrum(np.arange(25).reshape((5,5)))
>>> lum.to_array(L)
array([[ 0., 0., 1., 2., 3., 4.],
      [0., 0., 1., 2., 3., 4.],
      [1., 5., 6., 7., 8., 9.],
      [ 2., 10., 11., 12., 13., 14.],
      [ 3., 15., 16., 17., 18., 19.],
      [ 4., 20., 21., 22., 23., 24.]])
```

Module contents

Module contents

1.7 Changelog

All notable changes to this project will be documented in this file.

The format is based on Keep a Changelog, and this project adheres to Semantic Versioning.

1.7.1 2022-04-29 - version 0.2

Added

- Set up read the docs documentation
- Added metadata convention
- Add proper handling of variance on Jacobian transformation during axis conversion (eV, invcm)

Changed

- Account for the general availability of non-uniform axes with the HyperSpy v1.7 release
- Make LumiTransient 1D and add 2D LumiTransientSpectrum class
- Add python 3.10 build. Remove python 3.6.
- Fix error in background dimensions that allows compatibility for updated *map* in HyperSpy (failing integration tests)
- Fix for links in PyPi
- Deprecate *exposure* argument of *s.scale_by_exposure* in favor of *integration_time* in line with metadata convention
- Add deprecation warning to remove_background_from_file

1.7.2 2021-11-23 - version 0.1.3

Changed

- Mentions of the now deleted non_uniform_axes branch in HyperSpy updated to RELEASE_next_minor
- Change 'master' to 'main' branch
- Updated/corrected badges and other things in README.md and other documentation files

1.7.3 2021-08-22 - version 0.1.2

Added

- This project now keeps a Changelog
- · Added signal-hierarchy for time-resolved luminescence
- Added GitHub action for release
- Created logo

Changed

- Consistent black-formatting
- fixed join_spectra
- fixed tests

1.7.4 2021-03-26 - version 0.1

Added

• The first release, basic functionality implemented

1.8 Citing LumiSpy

LumiSpy is maintained by an active community of developers.

If LumiSpy has been significant to a project that leads to an academic publication, please acknowledge that fact by citing it. The DOI in the badge below is the Concept DOI – it can be used to cite the project without referring to a specific version. If you are citing LumiSpy because you have used it to process data, please use the DOI of the specific version that you have employed. You can find it by clicking on the DOI badge below:

1.9 Contributing

LumiSpy is meant to be a community maintained project. We welcome contributions in the form of bug reports, documentation, code, feature requests, and more. In the following we refer to some resources to help you make useful contributions.

1.9.1 Issues

The issue tracker can be used to report bugs or propose new features. When reporting a bug, the following is useful:

- give a minimal example demonstrating the bug,
- copy and paste the error traceback.

1.9.2 Pull Requests

If you want to contribute to the LumiSpy source code, you can send us a pull request. Small bug fixes are corrections to the user guide are typically a good starting point. But don't hesitate also for significant code contributions - if needed, we'll help you to get the code ready to common standards.

Please refer to the HyperSpy developer guide in order to get started and for detailed contributing guidelines.

The kikuchypy contributors guide, another HyperSpy extension, also is a valuable resource that can get you started and provides useful guidelines.

Reviewing

As quality assurance, to improve the code, and to ensure a generalized functionality, pull requests need to be thoroughly reviewed by at least one other member of the development team before being merged.

1.9.3 Documentation

The LumiSpy documentation consists of three elements:

- Docstrings following the numpy standard that document the functionality of individual methods on GitHub.
- The documentation written using Sphinx and hosted on Read the Docs. The source is part of the GitHub repository.
- A set of curated Jupyter notebooks in the LumiSpy demos repository on GitHub that provide tutorials and example workflows.

Improving documentation is always welcome and a good way of starting out to learn the GitHub functionality. You can contribute through pull requests to the respective repositories.

1.9.4 Code style

LumiSpy follows Style Guide for Python Code with The Black Code style.

For docstrings, we follow the numpydoc standard.

Package imports should be structured into three blocks with blank lines between them:

- standard libraries (like os and typing),
- third party packages (like numpy and hyperspy),
- and finally lumispy imports.

1.9.5 Writing tests

All functionality in LumiSpy is tested via the pytest framework. The tests reside in the test directory. Tests are short methods that call functions in LumiSpy and compare resulting output values with known answers. Please refer to the HyperSpy development guide for further information on tests.

1.9.6 Releasing a new version

LumiSpy versioning follows semantic versioning and the version number is therefore a three-part number: MA-JOR.MINOR.PATCH. Each number will change depending on the type of changes according to the following:

- MAJOR increases when making incompatible API changes,
- MINOR increases when adding functionality in a backwards compatible manner, and
- PATCH increases when making backwards compatible bug fixes.

The process to release a new version that is pushed to PyPI and Conda-Forge is documented in the Releasing guide.

1.10 License

LumiSpy is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License (GPL) as published by the Free Software Foundation, either version 3 of the license, or (at your option) any later version.

LumiSpy is distributed in the hope that it will be useful, but **without any warranty**; without even the implied warranty of **merchantability** or **fitness for a particular purpose**. See the GNU General Public License for more details.

BIBLIOGRAPHY

- [Peck] E.R. Peck and K. Reeder, J. Opt. Soc. Am. 62, 958 (1972). doi:10.1364/JOSA.62.000958
- [Mooney] J. Mooney and P. Kambhampati, The Journal of Physical Chemistry Letters 4, 3316 (2013). doi:10.1021/jz401508t
- [Wang] Y. Wang and P. D. Townsend, J. Luminesc. 142, 202 (2013). doi:10.1016/j.jlumin.2013.03.052

PYTHON MODULE INDEX

lumispy, 27 lumispy.signals, 23 lumispy.signals.cl_spectrum, 13 lumispy.signals.common_luminescence, 15 lumispy.signals.common_transient, 16 lumispy.signals.el_spectrum, 17 lumispy.signals.luminescence_spectrum, 17 lumispy.signals.luminescence_transient, 22 lumispy.signals.luminescence_transientspec, 23 lumispy.signals.pl_spectrum, 23 lumispy.utils, 27 lumispy.utils.axes, 23 lumispy.utils.io, 25

INDEX

Symbols

_make_signal_mas	k()		<i>(lu-</i>	LazyCLSEMSpectru	ım
mispy.signa	als.cl_spectrum. (CLSpectrum		mispy.sign	als.cl_s
method), 1-	4			LazyCLSpectrum(a	class in l
_n_air() (in modul	e lumispy.utils.ax	xes), 23		15	
_reset_variance_	linear_model(Э	<i>(lu-</i>	LazyCLSTEMSpect	rum
mispy.signa	als.luminescence	_spectrum.L	umiSpeci	trum mispy.sign	als.cl_s
method), 1	7			LazyELSpectrum(a	class in l
•				17	
A				LazyLumiSpectrum	n
axis2eV()(in modu	le lumispy.utils.	axes), 23		mispy.sign	als.lumi
<pre>axis2invcm() (in n</pre>	iodule lumispy.ut	tils.axes), 23		LazyLumiTransier	ιt
•				mispy.sign	als.lumi
C				LazyLumiTransier	ntSpect
CLSEMSpectrum (<i>cl</i>	ass in lumispy.si	gnals.cl spe	ectrum),	mispy.sign	als.lumi
13	1.7			23	
CLSpectrum (<i>class i</i>	n lumispy.signal:	s.cl spectrui	n). 13	LazyPLSpectrum(a	class in l
CLSTEMSpectrum(c	lass in lumispy.si	gnals.cl spe	ectrum).	23	
13	I J	5	,,	LumiSpectrum	(<i>c</i> .
CommonLumi	(class	in	lu-	- mispy.sign	als.lumi
mispy.signa	als.common lum	inescence),	15	lumispy	
CommonTransient	(class	in	lu-	module, 27	
migny sign	als common trav	signt) 16		lumisny signals	

mispy.signals.common_transient), 16lumispy.signalscorrect_grating_shift()(lu-module, 23mispy.signals.cl_spectrum.CLSEMSpectrumlumispy.signals.cl_spectrummethod), 13module, 13crop_edges() (lumispy.signals.common_luminescence.Communicationscommon_luminescence

method), 15

D

data2eV() (in module lumispy.utils.axes), 23
data2invcm() (in module lumispy.utils.axes), 24

Е

ELSpectrum (*class in lumispy.signals.el_spectrum*), 17 eV2nm() (*in module lumispy.utils.axes*), 24

I

invcm2nm() (in module lumispy.utils.axes), 24

J

join_spectra() (in module lumispy.utils.axes), 24

L

(class luin pectrum), 15 umispy.signals.cl_spectrum), (class in lupectrum), 15 umispy.signals.el_spectrum), (class in luinescence_spectrum), 17 (class luin inescence_transient), 22 trum (class in luinescence_transientspec), lumispy.signals.pl_spectrum), lass in luinescence_spectrum), 17 lumispy.signals module, 23 lumispy.signals.cl_spectrum module, 13 module, 15 lumispy.signals.common_transient module, 16 lumispy.signals.el_spectrum module, 17 lumispy.signals.luminescence_spectrum module, 17 lumispy.signals.luminescence_transient module, 22 lumispy.signals.luminescence_transientspec module, 23 lumispy.signals.pl_spectrum module, 23 lumispy.utils module, 27

lumispy.utils.axes			
module, 23			
lumispy.utils.io			
module, 25			
LumiTransient	(class	in	lu-
mispy.signals.	luminescence	e_transient), 2	2
LumiTransientSpect	rum (cl	ass in	lu-
mispy.signals.	luminescence	e_transientspe	c),
23			

Μ

```
module
    lumispy, 27
    lumispy.signals, 23
    lumispy.signals.cl_spectrum, 13
    lumispy.signals.common_luminescence, 15
    lumispy.signals.common_transient, 16
    lumispy.signals.el_spectrum, 17
    lumispy.signals.luminescence_spectrum, 17
    lumispy.signals.luminescence_transient,
        22
    lumispy.signals.luminescence_transientspec,
        23
    lumispy.signals.pl_spectrum, 23
    lumispy.utils, 27
    lumispy.utils.axes, 23
    lumispy.utils.io, 25
```

Т

V

var2eV() (in module lumispy.utils.axes), 25
var2invcm() (in module lumispy.utils.axes), 25

Ν

Ρ

PLSpectrum (class in lumispy.signals.pl_spectrum), 23 px_to_nm_grating_solver() (lumispy.signals.luminescence_spectrum.LumiSpectrum method), 17

R

remove_background_from_file() (lumispy.signals.luminescence_spectrum.LumiSpectrum method), 18 remove_negative() (lumispy.signals.common_luminescence.CommonLumi method), 16 remove_spikes() (lumispy.signals.cl_spectrum.CLSpectrum method), 14

S

savetxt() (in module lumispy.utils.io), 25