Data analysis for EELS and CL using HyperSpy

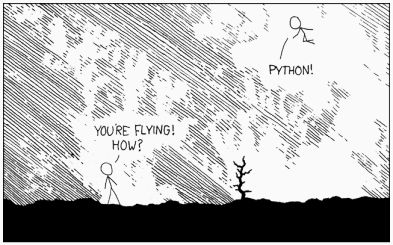
Jonas Lähnemann, Sean Collins, Kagiso Loeto, Domenik Spallek, Aidan Campbell,
... and the HyperSpy, LumiSpy and eXSpy developers

eBEAM 2024 – School on Nano-optics with Free Electrons, Aussois, September 04, 2024

Today: Introductory lecture – complemented by interactive tutorials in small groups

Why use python for scientific data analysis?

- Both a genuine programming and a scripting language
- Free as in speech (open source) and as in beer (no fees)
- Portable: Runs on any environment (Win, Mac, Linux)
- Intuitive and readable code
- Reproducible and reusable analysis routines



Courtesy of XKCD: https://xkcd.com/353/

python™

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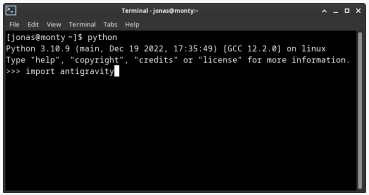
- Different environments
  - Use interactive console: `python`, `ipython`
  - Run script files: `python silly-walk.py`
  - Matlab-style integrated desktop environments: e.g. `spyder`
  - Mathematica-style notebooks: `Jupyter`
  - Dedicated frontends: e.g. `hyperspyUI`



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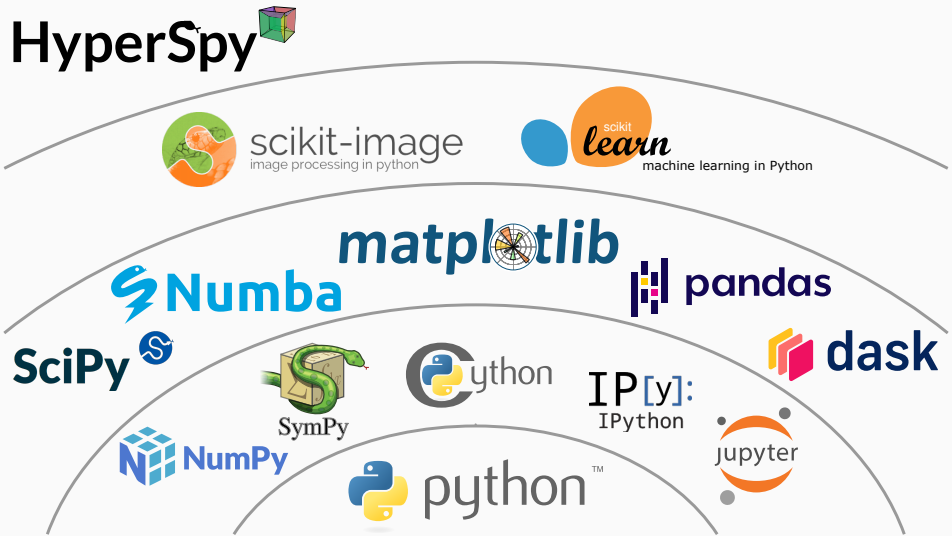
- Different environments
- Vast and unmatched range of scientific libraries:
  - `numpy` + `scipy` + `matplotlib` = Matlab replacement
  - `SymPy`, `scikit-image`, `scikit-learn`, ...

The scientific python stack



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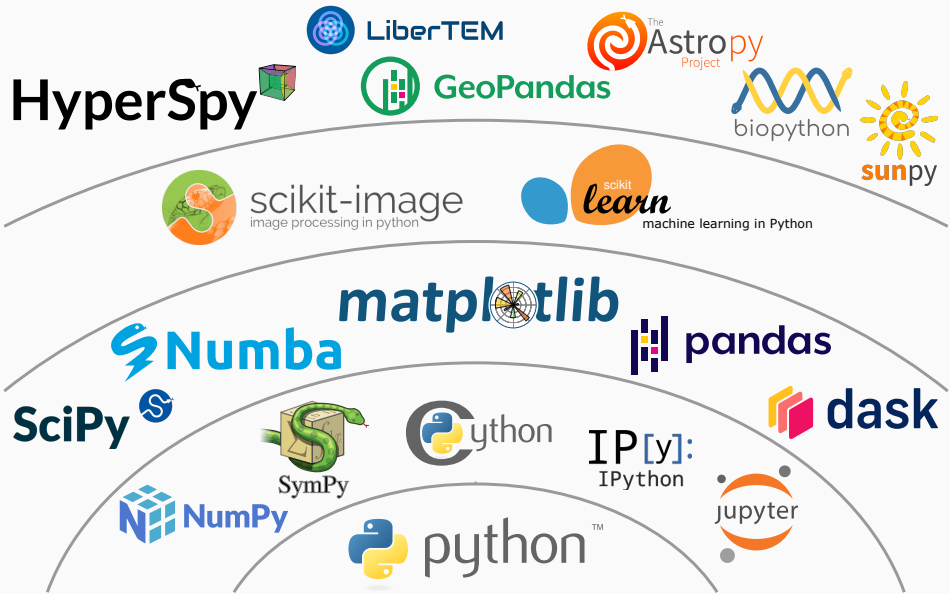
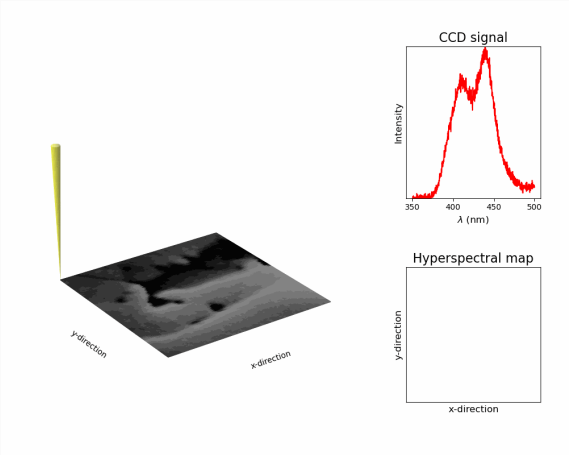


What is HyperSpy?

- Open-source `python` library for interactive **analysis of multi-dimensional data**
- Easily extend operations from a single spectrum/image to multi-dimensional arrays



HyperSpy

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- Easy access to cutting-edge signal processing tools

```
s = hs.load('beautiful-plumage.hspy')
m = s.create_model()
g = hs.model.components1D.GaussianHF()
m.append(g)
m.multifit()
```

HyperSpy

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- Community-driven: Developed by scientists for scientists
- Vibrant and welcoming community of developers and users committed to well-documented, powerful and easy-to-use toolbox

Francisco de la Peña 😇
Pierre Burdet
Magnus Nord
Mike Sarahan
Vadim Migunov
Timothy Poon
Suhas Somnath

Eric Prestat
Petras Jokubauskas
Tomas Ostasevicius
Joshua Taillon 👋
Alberto Eljarrat
Stefano Mazzucco
Tom Slater

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Tom Furnival
Katherine MacArthur
Thomas Aarholt
Jan Caron
Nicolas Tappy
Michael Walls

Jonas Lähnemann
Carter Francis
Duncan N. Johnstone
Paul Quinn
Takashi Nemoto
Niels Cautaerts
Hugh Ramsden

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- Mature and robust code base
- Ecosystem: Extension framework for different signal types

HyperSpy

A brief history of HyperSpy?

- 2007-2012: Developed by Francisco de la Peña in his PhD (Univ. Paris-Sud) as EELSlab
- 2010: Open-sourced on GitHub and renamed to HyperSpy
- 2016: Migration to python 3 (with version 0.8.4) and release of version 1.0
- 2019: Introduction of extension mechanism (with version 1.5)
- 2023: Version 2.0 released – I/O and domain-specific functions split out

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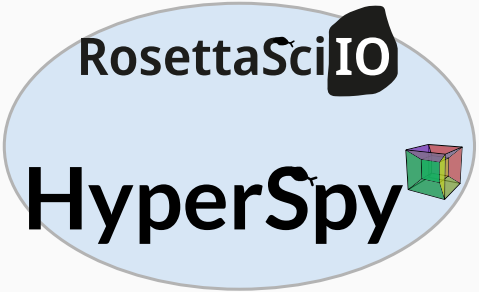
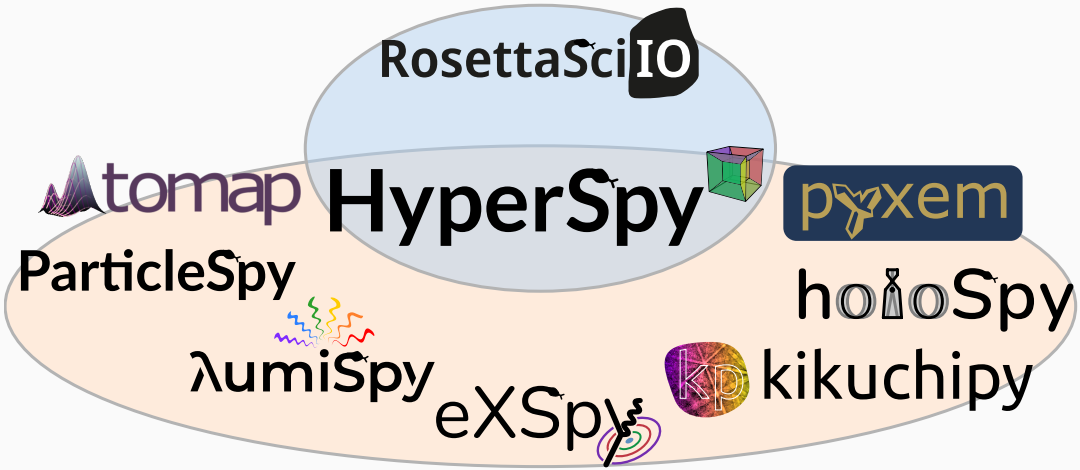
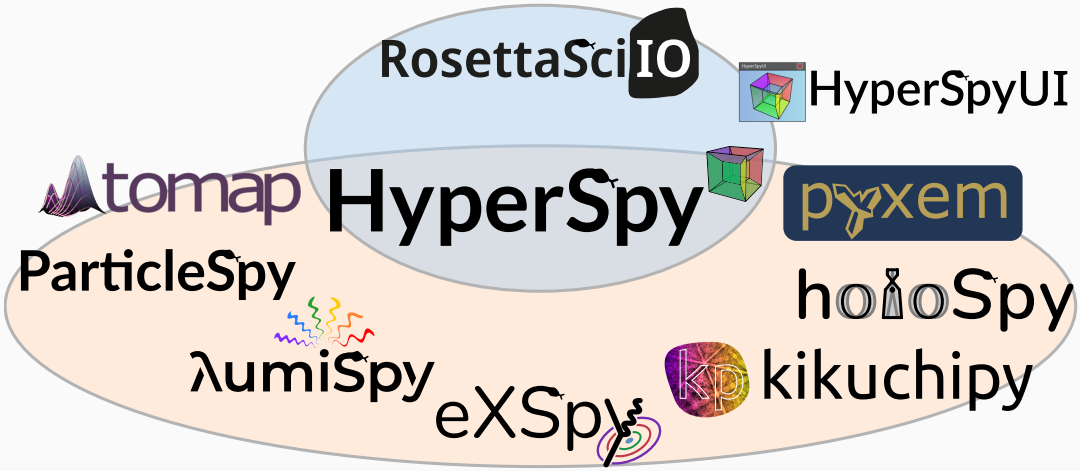
- 2023: Version 2.0 released – I/O and domain-specific functions split out
- Now ...
  - $>$ 1200 citations (google scholar)
  - 56 releases
  - 70 contributors
  - $>$ 90k lines of code (excluding extensions)
  - $>$ 500 stars on GitHub (users with GitHub account)
  - used in $>$ 200 other GitHub projects
  - ... and still growing!

HyperSpy 

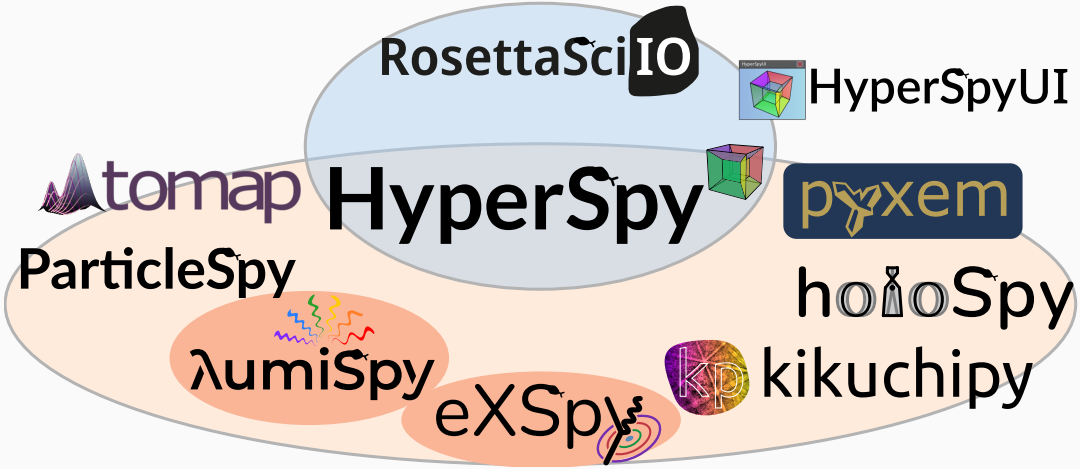

RosettaSciIO
HyperSpy


RosettaSciIO
tomap
HyperSpy
pyxem
ParticleSpy
holoSpy
λumiSpy
eXSpy
kikuchipy

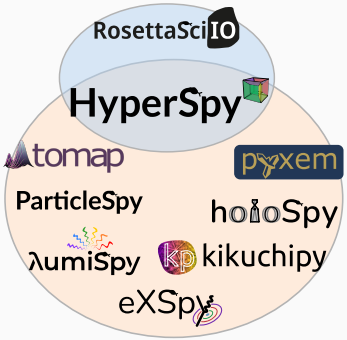
The HyperSpy ecosystem (v2.0)



The HyperSpy ecosystem (v2.0)



The HyperSpy ecosystem: Extensions



- `RosettaSciIO`: Reading and writing scientific data formats

Domain specific:

- `eXSpy`: Energy Dispersive X-ray Spectroscopy (EDS) and Electron Energy Loss Spectroscopy (EELS)
- `LumiSpy`: Luminescence spectroscopy
- `pyxem`: 4D Scanning Transmission Electron Microscopy (STEM)
- `kikuchipy`: Electron Backscatter Diffraction (EBSD) patterns
- `holospy`: Off-axis Electron Holography
- `Atomap`: Atomic resolution STEM
- `ParticleSpy`: Segmentation and analysis of nanoparticles

- `HyperSpyUI`: User Interface (limited functionality)

HyperSpy features include

- Tools for loading/saving various data file formats (`RosettaSciIO`)
- Analytical tools that exploit the multidimensionality of datasets
- Data visualization: evaluate datasets during the analysis, provide interactive operation for certain functions, and plotting
- Efficient handling of big datasets ("lazy" and parallel processing)
- Extracting subsets of data from multidimensional datasets: regions of interest and a powerful numpy-style indexing mechanism
- Handling of non-uniform data axes
- User-friendly and powerful framework for multidimensional model fitting: provides many standard functions, easily extended to custom ones
- Machine learning algorithms, useful for e.g. denoising data, decomposition

HyperSpy 

Selection of supported data formats

For saving analyses, **RosettaSciIO** provides dedicated hdf5-based `.hspy` and compressible zarr `.zspy` data formats.

RosettaSciIO supports a wide range of microscopy (and spectroscopy) related file types.

All relevant formats for cathodoluminescence (CL) spectroscopy can be read:

- Attolight digital surface `.sur` (write support, limited `metadata` parsing)
- Delmic `.hdf5` (full parsing with next release)
- Gatan DigitalMicrograph `.dm3/.dm4`
- Horiba JobinYvon `.xml` (same metadata as binary `.l5s` or `.l6s`)

```
s = hs.load('spam-eggs-tofu.hspy')
```

RosettaSciIO

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Other relevant formats for luminescence spectroscopy:

- Hamamatsu streak camera images in `.img` or `.tif` format
- Renishaw wire format `.wdf`
- TriVista XML `.tvf`

```
s = hs.load('spam-spam-tofu.tif')
```

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Relevant formats for EDS and EELS include:

- MSA spectral file format `.msa` (write support)
- Bruker `.spx` (single spectrum) and `.bcf` (spectrum images)
- CEOS Panta Rhei `.prz` (EELS)
- EDAX `.spc` (single spectra) and `.spd` (EDS spectrum image)
- FEI TEM Imaging & Analysis `.ser` and `.emi` files (EELS & EDS spectra/spectrum images)
- Gatan DigitalMicrograph `.dm3/.dm4` (EELS)
- ThermoFisher Velox Electron Microscopy Dataset `.emd` (EDS spectrum images)

```
s = hs.load('spam-eggs-spam.msa')
```

RosettaSciIO

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RosettaSciIO supports a wide range of microscopy (and spectroscopy) related file types.

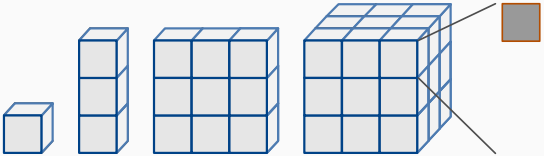
Generic data formats, such as NeXus HDF5 or many image formats are also supported.

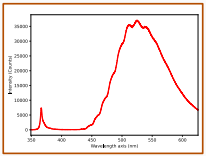
Common 4D-STEM datasets are supported for analysis with `pyxem`.

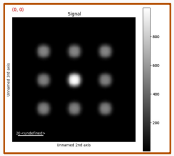
```
s = hs.load('spam-spam-spam.zspy')
```

RosettaSciIO

Core design principles: Navigation versus Signal dimensions







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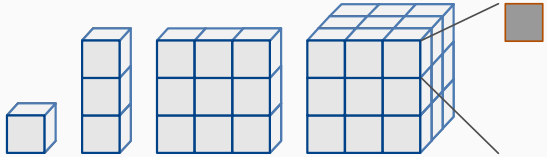
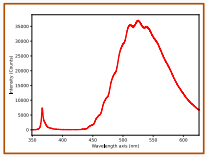
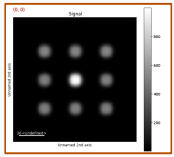
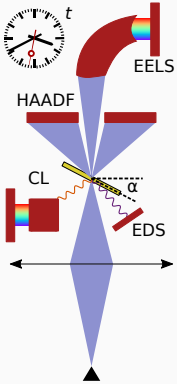








[Francisco de la Peña]

Technique	Dimensions Navigation | Signal	Total
HAADF	$(x, y\|)$ / $(\|x, y)$	2
Spectrum (CL, EDS, EELS)	$(\|E)$	1
Linescan (CL, EDS, EELS)	$(x\|E)$	2
Map (CL, EDS, EELS)	$(x, y\|E)$	3
Temperature series map (CL)	$(x, y, T\|E)$	4
Tilt series map (EELS)	$(x, y, \alpha\|E)$	4
Tilt and time series map (EELS)	$(x, y, \alpha, t\|E)$	5
Diffraction	$(x, y, \alpha, t\|x^*, y^*)$	6

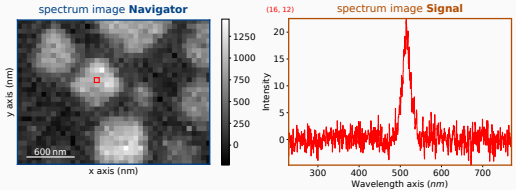
Core design principles: Navigation versus Signal dimensions

- Navigation and signal axes are interchangeable
- Transposing signal flips navigation and signal axes

The same 3D dataset can be represented as either:

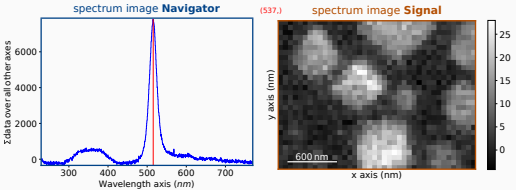
2D array of spectra
$(x, y|\lambda)$

```
cl1.plot()
```

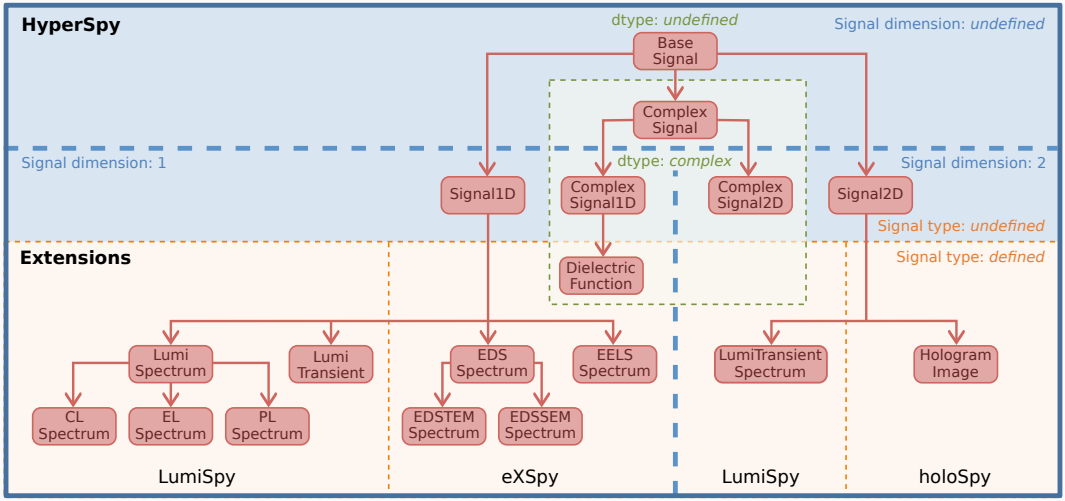


1D array of images
$(\lambda|x, y)$

```
cl1.T.plot()
```

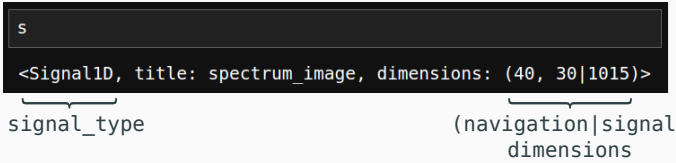


Core design principles: The HyperSpy `signal class` hierarchy



`subclasses` inherit functions & provide additional (datatype/domain-specific) features

Core design principles: HyperSpy signal object



- `Axes manager` – axes objects for each navigation and signal axis
- `Data` – multidimensional array
- `Metadata` – parsed information about measurement conditions, sample and file
- `(Original metadata)` – metadata tree as saved in vendor file

Core design principles: HyperSpy signal object

```
s

<Signal1D, title: spectrum_image, dimensions: (40, 30|1015)>
```

`signal_type` — `(navigation|signal) dimensions`

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```
s.axes_manager
```

< Axes manager, axes: (40, 30|1015) >

Navigation axis name	size	index	offset	scale	units
x	40	0	0.0	61.0	nm
y	30	29	0.0	61.0	nm
Signal axis name	**size**		**offset**	**scale**	**units**
Wavelength	1015		229.0	1.0	nm

Core design principles: HyperSpy signal object

```
s

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```

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```
s.data

array([[[-2.49761505e+00, -2.12892204e+00, -6.81961551e-01, ...,
          2.39770962e-01,  3.13369195e+00,  5.80652438e-01],
        [ 2.43140998e+00, -3.19181309e+00, -1.34478831e+00, ...,
         -1.91813092e-01,  1.34926127e+00,  4.33108368e-02],
        [-7.11180500e-01, -1.22476480e+00,  1.16721557e+00, ...,
          2.04561165e+00, -7.11180500e-01, -1.58957657e+00],
        ...,
```

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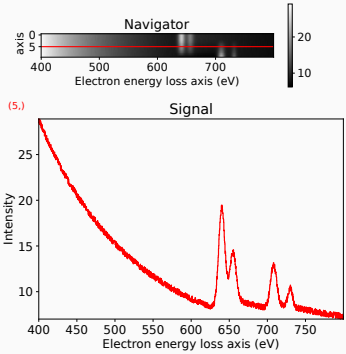
```
s.metadata

▼ Acquisition_instrument
  ▼ CCD
    ◦ amplification = 1
    ◦ binning = 1
    ◦ channels = 1024
    ◦ exposure_time_s = 0.05
  ▼ SEM
▼ General
  ▼ FileIO
    ▶ 0
    ▼ 1
      ◦ hyperspy_version = 2.2.0
      ◦ io_plugin = rsciio.hspy
      ◦ operation = load
```

Core design principles: numpy-style indexing

Simple syntax to select subsets of data in all dimensions:

```
s = exspy.data.EELS_MnFe()
s.plot()
```



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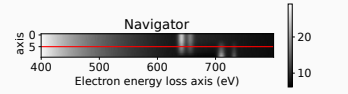
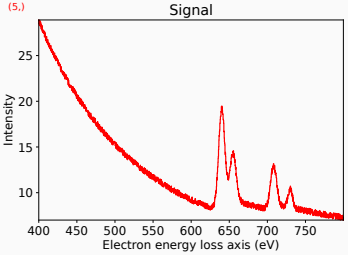
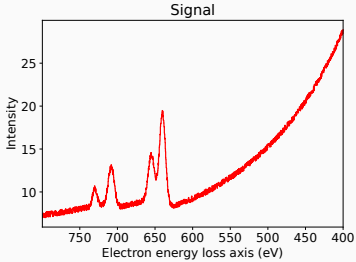




Select navigation `pixel 5` and invert signal axis:

```
s.inav[5].isig[::-1].plot()
```



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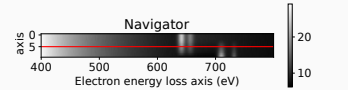
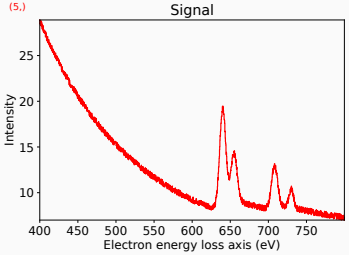
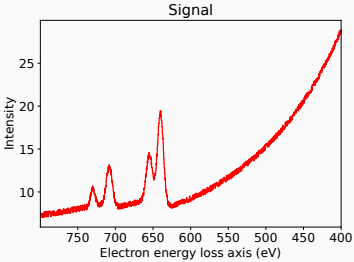
```





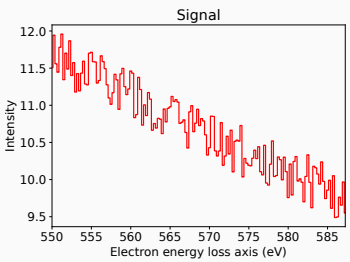
Select navigation `pixel 5` and invert signal axis:

```
s.inav[5].isig[::-1].plot()
```



Plot single spectrum signal range: `pixels 600-750`

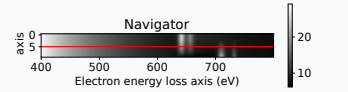
```
s.inav[5].isig[600:750].plot()
```

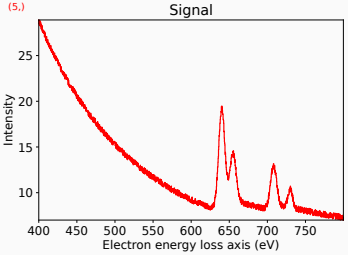


Core design principles: numpy-style indexing

Simple syntax to select subsets of data in all dimensions:

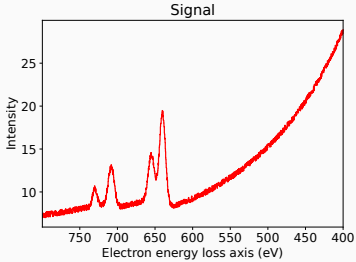
```
s = exspy.data.EELS_MnFe()
s.plot()
```





Select navigation `pixel 5` and invert signal axis:

```
s.inav[5].isig[::-1].plot()
```

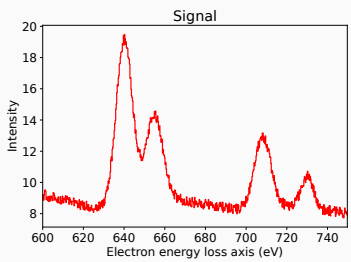


Plot single spectrum signal range: `pixels 600-750`

```
s.inav[5].isig[600:750].plot()
```

Plot single spectrum signal range: `600-750 eV`

```
s.inav[5].isig[600.:750.].plot()
```



What is eXSpy

- HyperSpy extension for EDS and EELS data
- The scientific domains at the roots of HyperSpy
- Adds signal-specific functions
- One of the most powerful HyperSpy extensions

eXSpy features include

- Specific signal types (python classes) for EDS and EELS
- Dedicated models to fit EDS and EELS spectra
- Database of X-ray energies
- EDS quantification (STEM only, not SEM)
- EELS: Supports different datasets for the Generalised Oscillator Strengths (GOS)
- EELS fine structure analysis

eXSpy

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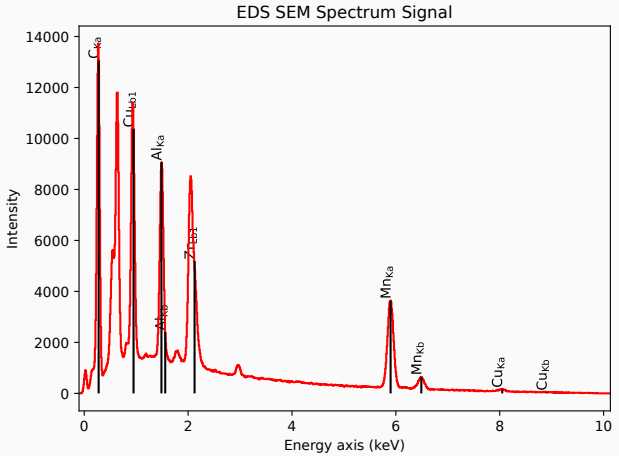
- EDS quantification (STEM only, not SEM)
- EELS: Supports different datasets for the Generalised Oscillator Strengths (GOS)
- EELS fine structure analysis
- All of the built-in HyperSpy tools!

eXSpy

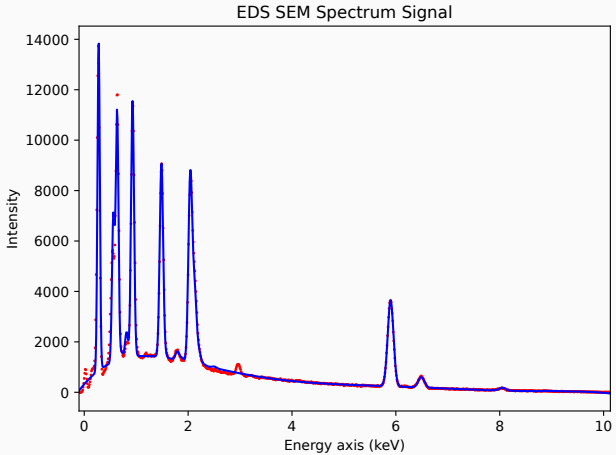
eXSpy examples: Labeling elements in plots

```
s = exspy.data.EDS_SEM_TM002()
s.add_elements(['C','Mn','Cu','Al','Zr'])
s.axes_manager[0].name = 'Energy'
s.plot(True, only_lines=['Ka','b'])
```



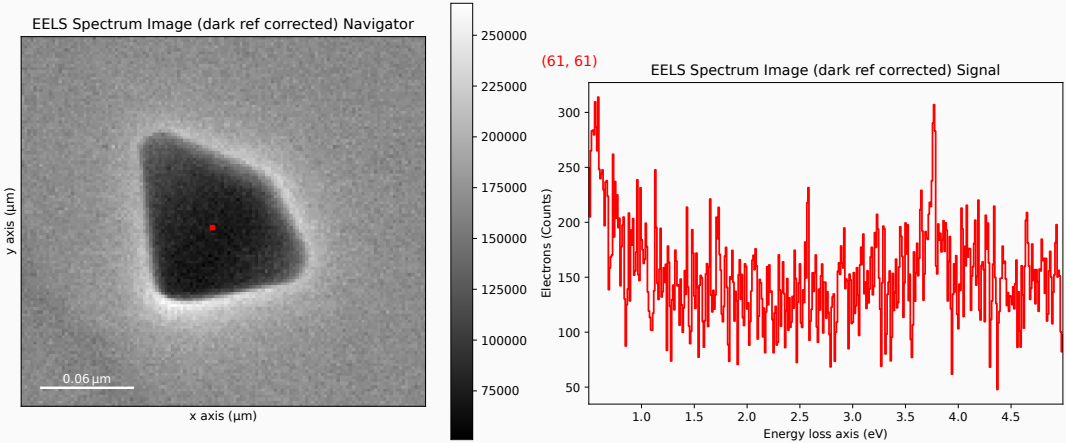
eXSpy examples: Using predefined model


```
m = s.create_model()
m.fit()
m.fit_background()
m.plot()
```



eXSpy examples: Signal decomposition using machine learning

Noisy, low-intensity EELS map:

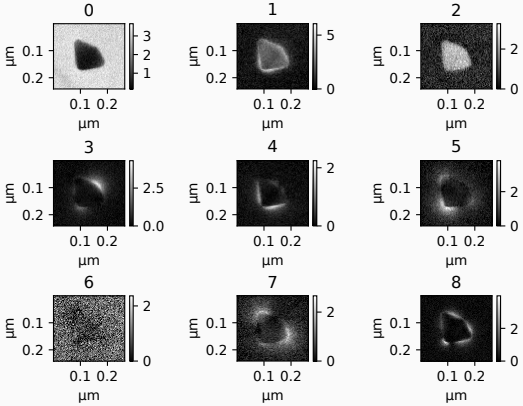


eXSpy examples: Signal decomposition using machine learning

e.g. Non-negative Matrix Factorisation (NMF): identify signal components and distribution

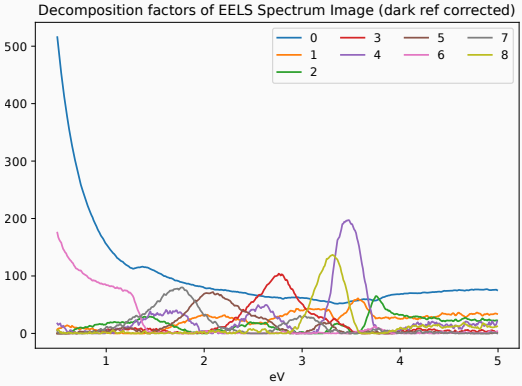
```
s.decomposition(normalize_poissonian_noise=True,algorithm='NMF',output_dimension=9)
s.plot_decomposition_loadings()
```

Decomposition loadings of EELS Spectrum Image (dark ref corrected)




```
s.plot_decomposition_factors()
```

Decomposition factors of EELS Spectrum Image (dark ref corrected)



What is LumiSpy

- `HyperSpy` extension for luminescence spectroscopy data
- Provides the framework to work with photoluminescence (PL), cathodoluminescence (CL), electroluminescence (EL) and Raman spectroscopy
- Adds signal-specific functions
- Work in progress … open for other contributors

λumiSpy

LumiSpy features include

- Specific signal types (python classes) for luminescence spectra and transients
- Transformation of wavelength to electron volt and wavenumbers/Raman shift (non-uniform signal axes)
- Tools such as data normalization/scaling, centre of mass
- Utility functions useful in luminescence spectroscopy data analysis: joining multiple spectra, unit conversion etc.

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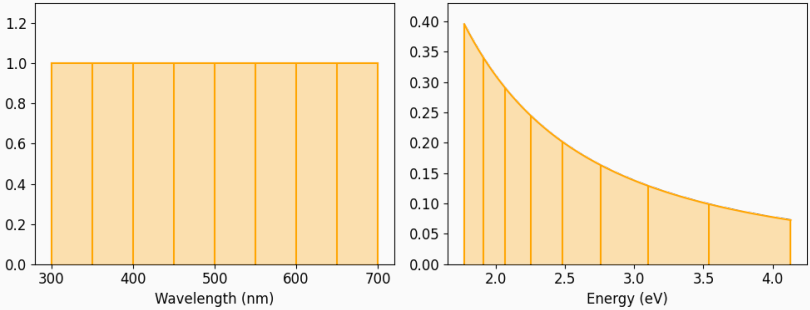
- Transformation of wavelength to electron volt and wavenumbers/Raman shift (non-uniform signal axes)
- Tools such as data normalization/scaling, centre of mass
- Utility functions useful in luminescence spectroscopy data analysis: joining multiple spectra, unit conversion etc.
- All of the built-in HyperSpy tools!

Jacobian Transformation: Wavelength → Energy axis

Preserve integral under function $I(E)dE = I(\lambda)d\lambda$

after non-uniform axis transformation $E = hc/\lambda$

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



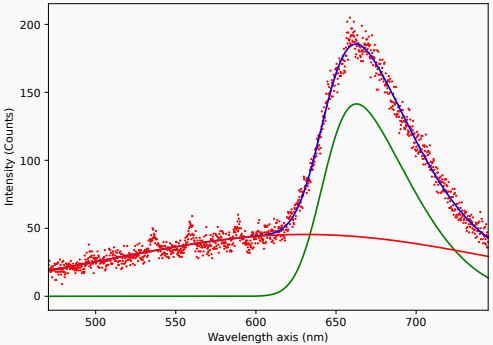

```
s.to_eV()
```

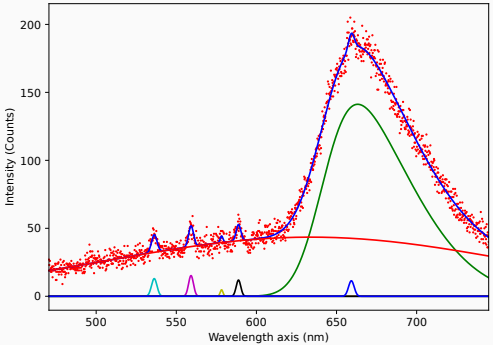
[J. Mooney and P. Kambhampati, The Journal of Physical Chemistry Letters 4, 3316 (2013). doi:10.1021/jz401508t]
[Y. Wang and P. D. Townsend, J. Luminesc. 142, 202 (2013). doi:10.1016/j.jlumin.2013.03.052]

LumiSpy examples: Scripted fitting of a complex model

CL spectrum of luminescent centers in h-BN on SiO_2

- SiO_2 emission: broad Gaussian & skew normal distribution
- Automatically identify sharp peaks in spectrum and add additional Gaussian peaks





[Hernández-Mínguez et al., Phys. Rev. Appl. 10, 2331 (2018)]

LumiSpy examples: Scripted fitting of a complex model

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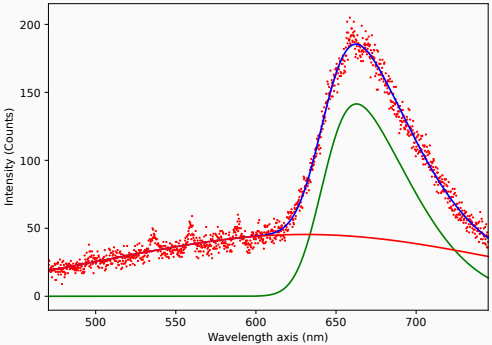
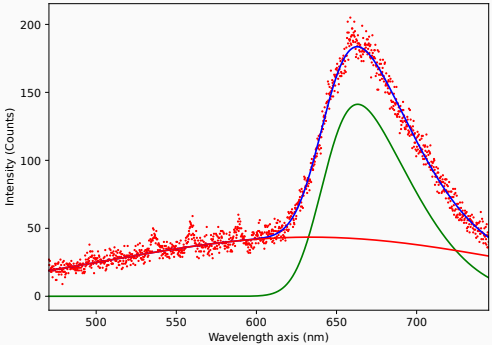
- Yields refined background spectrum



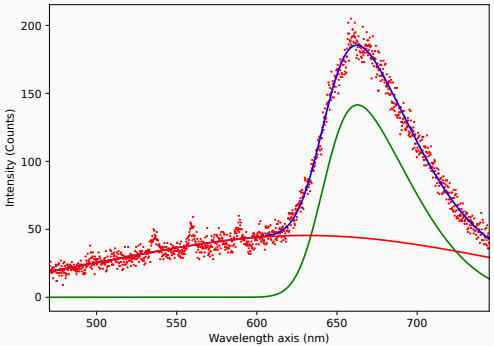


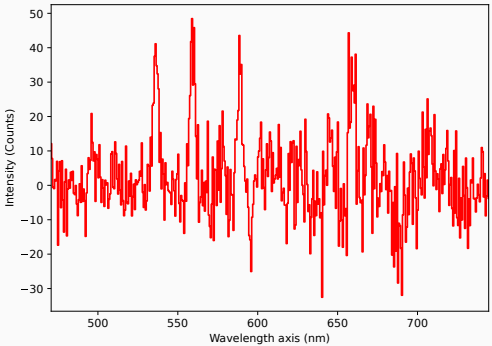
[Hernández-Mínguez et al., Phys. Rev. Appl. 10, 2331 (2018)]

LumiSpy examples: Scripted fitting of a complex model

CL spectrum of luminescent centers in h-BN on SiO_2

- SiO_2 emission: broad Gaussian & skew normal distribution
- Automatically identify sharp peaks in spectrum and add additional Gaussian peaks
- Yields refined background spectrum, which can then be subtracted

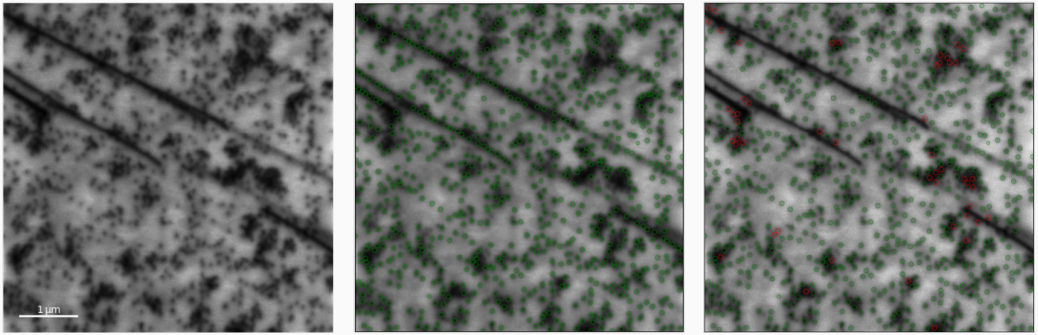




[Hernández-Mínguez et al., Phys. Rev. Appl. 10, 2331 (2018)]

LumiSpy examples: Dislocation density in (In,Ga)N layers

- Panchromatic CL maps show dislocations as dark spots
- Automated spot identification using Laplacian of Gaussian algorithm
- Manual optimization

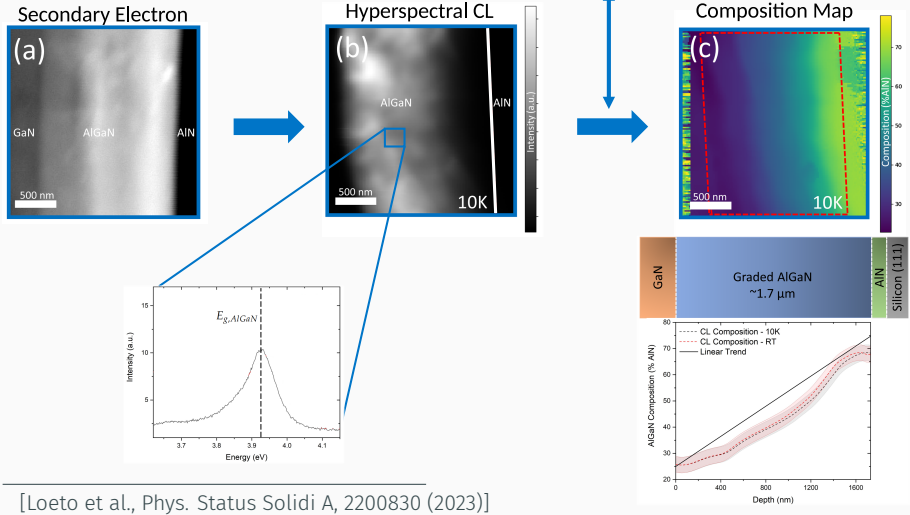


$N_{TD} = 860, \rho_{TD} = 2.56 \times 10^9$ cm^{-2}

[Campbell, Master thesis, Strathclyde Univ. (2024)]

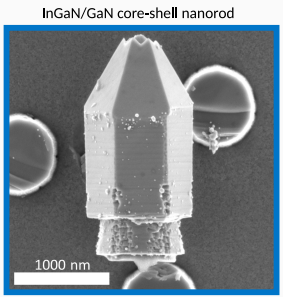
LumiSpy examples: Quantifying alloy composition of graded (Al,Ga)N buffer

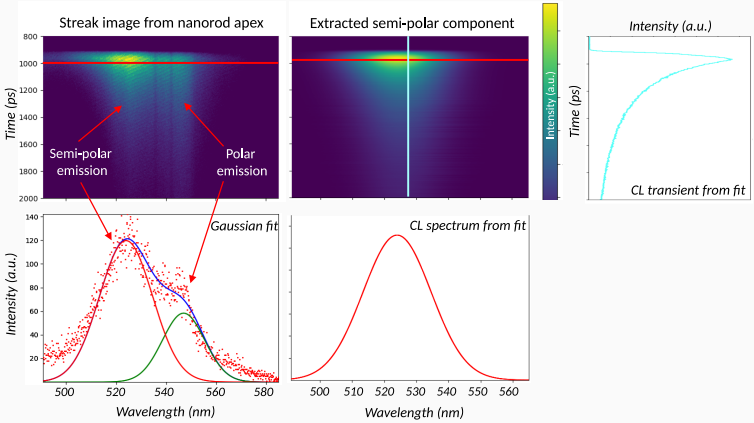
$$E_{g,AlGaN} = xE_{g,AlN} + (1-x)E_{g,GaN} - bx(1-x)$$



[Loeto et al., Phys. Status Solidi A, 2200830 (2023)]

LumiSpy examples: Separating emission bands from streak-camera data





[Loeto et al., Nanotechnology, under review (2024)]

The community: Resources – getting started and obtaining help

HyperSpy

- Website: https://hyperspy.org
- User guide: https://hyperspy.org/hyperspy-doc/current
- Tutorial notebooks: https://github.com/hyperspy/hyperspy-demos
- Gitter chat: https://gitter.im/hyperspy/hyperspy

LumiSpy

- User guide: https://lumispy.org
- Tutorial notebooks: https://github.com/LumiSpy/lumispy-demos

eXSpy

- User guide: https://hyperspy.org/exspy
- Tutorial notebooks: https://github.com/hyperspy/exspy-demos

The community: Contributing

Anyone can make LumiSpy/eXSpy/HyperSpy better! Don't be shy!

- Community-driven development
- Report bugs on the github issue tracker
- Improve documentation
- Help review pull requests on github
- Contribute new functionalities:
  - Include tests and documentation
  - More effort than scripting for personal use
  - \+ Shared development (avoid reinventing the wheel)

Cite HyperSpy and its extensions

HyperSpy, LumiSpy and eXSpy have DOIs provided by Zenodo. There is a generic DOI for the whole project, but every version automatically gets a dedicated DOI assigned.

Getting started for Tutorials

Interactive tutorial presented as Jupyter Notebook – Follow on your own Laptop!

You will be grouped based on prior knowledge (self-assessment).

1. Install python and relevant libraries on your Laptop:

- We recommend installing the `HyperSpy Bundle`
- If you already have python installed, get the following packages from `pip` or `conda`:
  - `hyperspy, lumispy, exspy, hyperspy-gui-ipywidgets, scikit-learn`
- See also Installation Guides at https://lumispy.org and https://hyperspy.org
- A number of colleagues here can help you in the coffee breaks to get started!

2. Get the demo notebooks and data:

- https://github.com/lumispy/eBEAM2024-Tutorial

PS: Find this presentation and relevant links in the above github repository!