OPEN-SOURCE FOR RAMAN SPECTROSCOPY HARMONISATION

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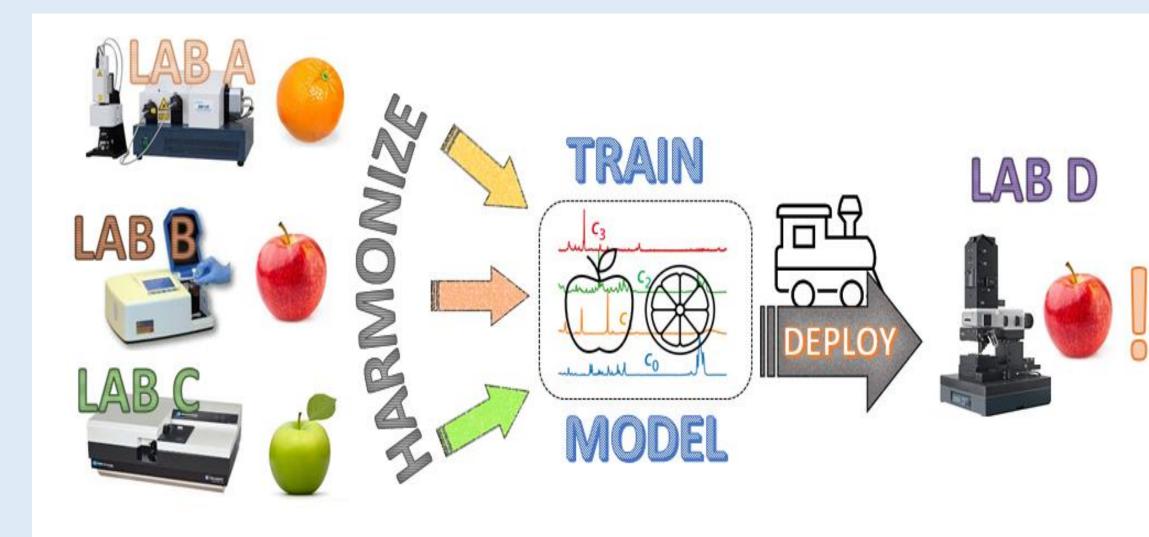
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BACKGROUND MOTIVATION AND OBJECTIVE

- Raman spectroscopy is becoming a key technology used in the research and development for characterization of materials.
- Ideally, spectra should be comparable and linked to specific material properties.
- In real life, Raman spectra differ between instruments and depend on the spectrometer, optical path, or sample environment, among others, and only a limited number of calibration standards for Raman spectroscopy are available to date [1]



The CHARISMA EU's Horizon 2020 project aims to

- harmonize and standardize characterization by Raman spectroscopy
- including hardware, measurement protocols, and in-silico methods
- enabling end users to share digital spectral data through a FAIR database across domains and across the entire life cycle of diverse products

METHODS

Oranchada Easy

Oranchada Pro

We present **ramanchada2**, an open-source, MIT-licensed, Python package https://github.com/h2020charisma/ramanchada2

Ramanchada2 is published at the Python Package Index repository (PyPI).

Raman spectra data input and output

✓ Multiple file formats supported

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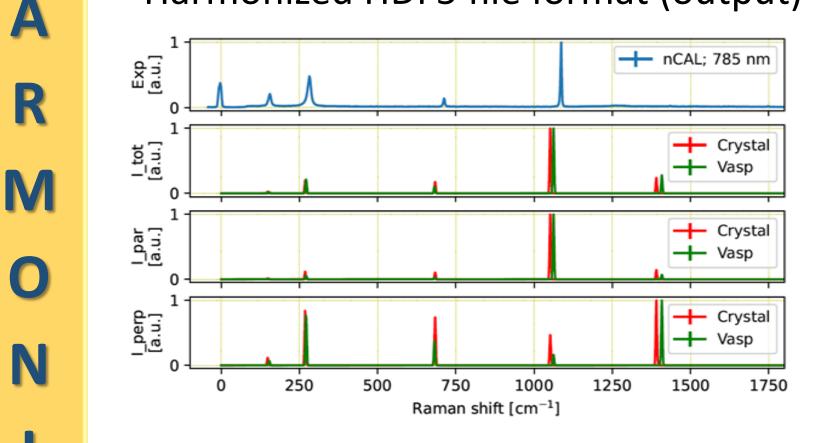
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✓ Simulated data (VASP, Crystal) Harmonized HDF5 file format (output)



Spectra preprocessing

Scale & normalize x-axis ✓ Baseline removal

✓ Resampling non-uniform DFT

Find peak candidates

- ✓ Sharpening
- ✓ Bayesian Gaussian mixtures
- ✓ Peak finding

Peak fitting

800

0.75 -

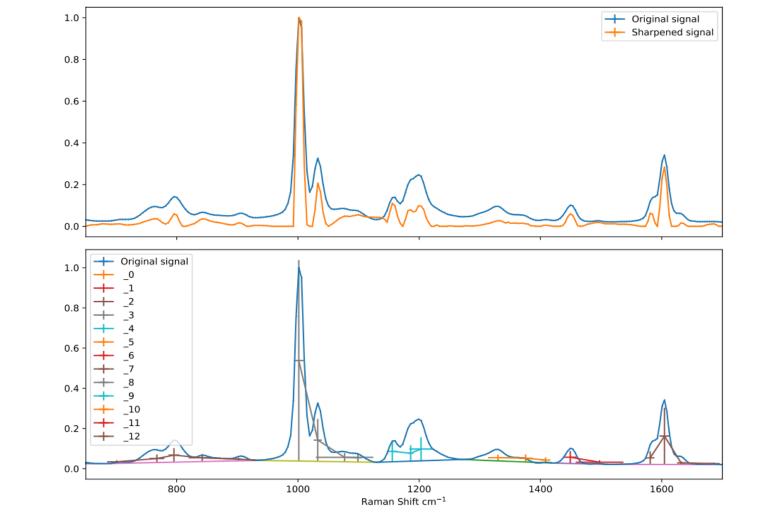
Special pages

✓ Composite model

Pearson, Moffat

 \checkmark Fit on sections

✓ Group overlapping peaks



✓ Models available: Gaussian, Voigt,

Initial guess

Best fit

Best fit components

1200

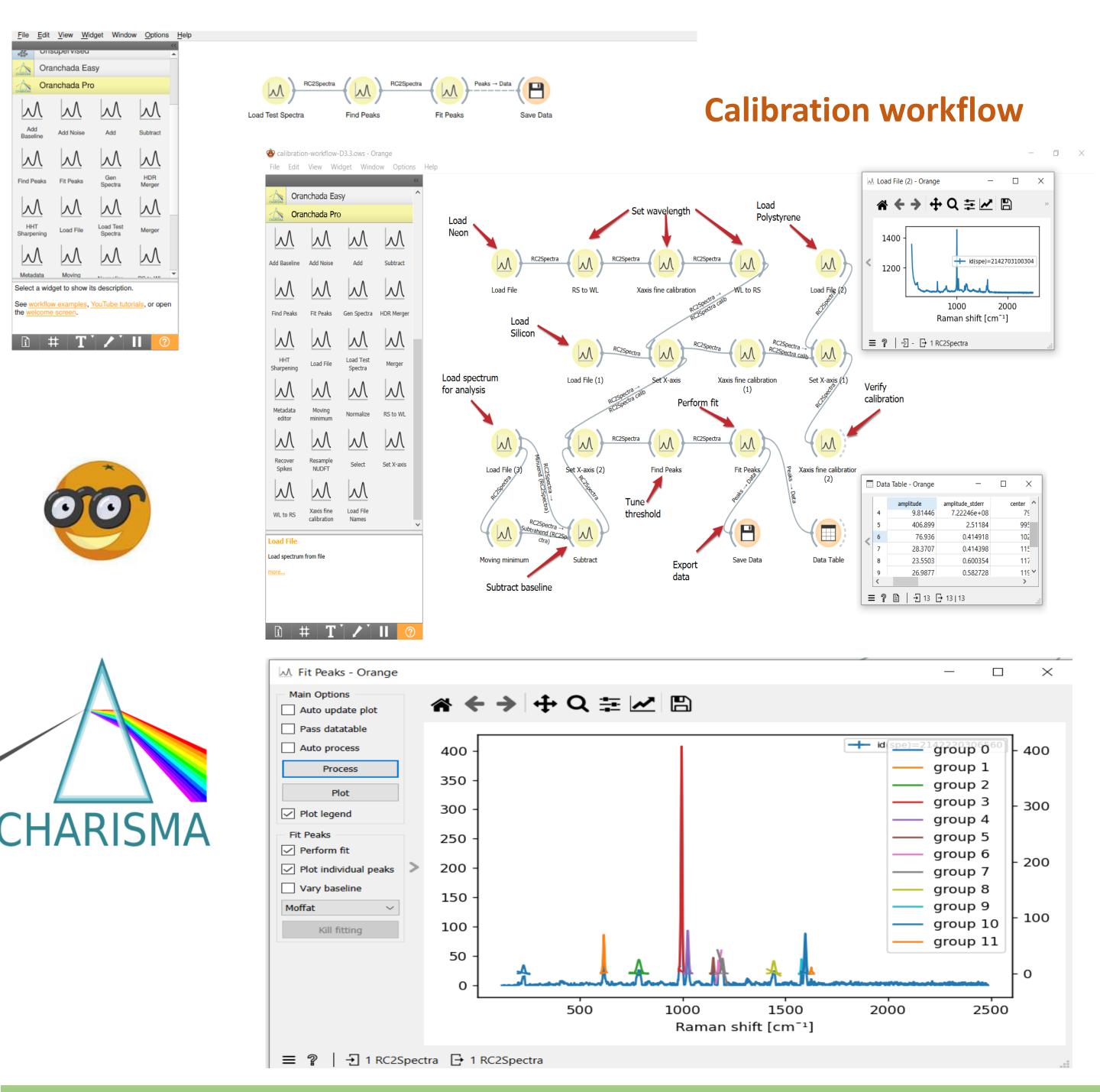
Raman Shift cm⁻¹

Original signa

-+- Original signa

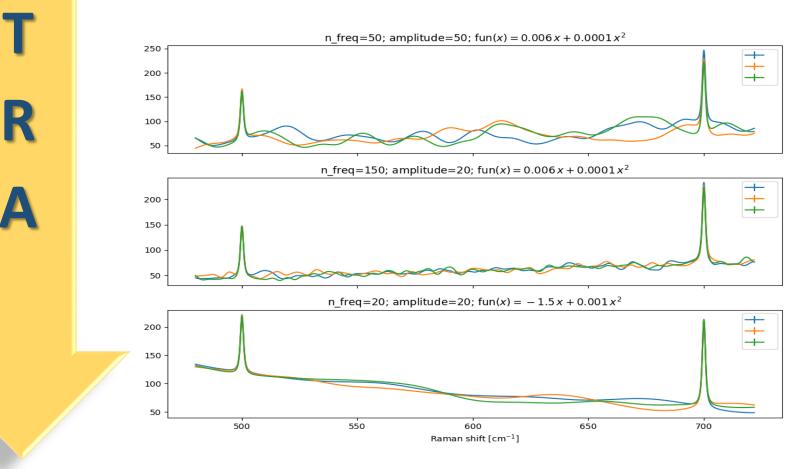
Original signa

To facilitate Raman spectra analysis for the end users, we are developing **Oranchada**, an user friendly wrapper of all ramanchada2 functionality, which is available for installation as an add-on of the popular **Orange data mining software** [2]. The Oranchada package is also open source and MIT-licensed and actively developed at https://github.com/h2020charisma/oranchada.



spe deltas = rc2.spectrum.from delta lines(deltas={800:1e3, 1800:1.5e3, 2500:1e3}) eltas.resample NUDFT filter(xnew bins=100).convolve(lineshape='voigt', sigma=.1, gamma=1) initial.add baseline(n freq=30, amplitude=50, pedestal=10, func=**lambda** x: x*.05 - .00001*x**2) pe baseline.add poisson noise(scale=.5) spe complete.scale xaxis fun(lambda x: x**2*.0001 + x*.22) spe nobaseline = spe scaled.subtract moving minimum(6) spe resampled = spe nobaseline.resample NUDFT filter(xnew bins=100, x range=(0, 2500)) spe normalized = spe resampled normalized

- Synthetic spectra generation
- \checkmark User defined peaks (position, intensities)
- Convolve with peak profiles (Voigt, Gaussian, Pearson IV, VII, Moffat, User defined function)
- ✓ Add artificial baseline, noise



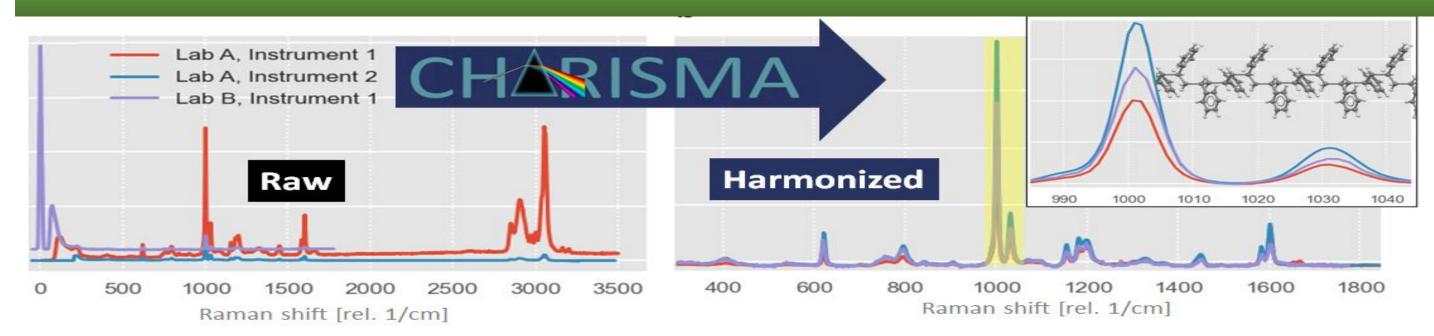
FAIR data (eNanoMapper compatible) raw and harmonized spectra

Wikibase for terminology harmonisation

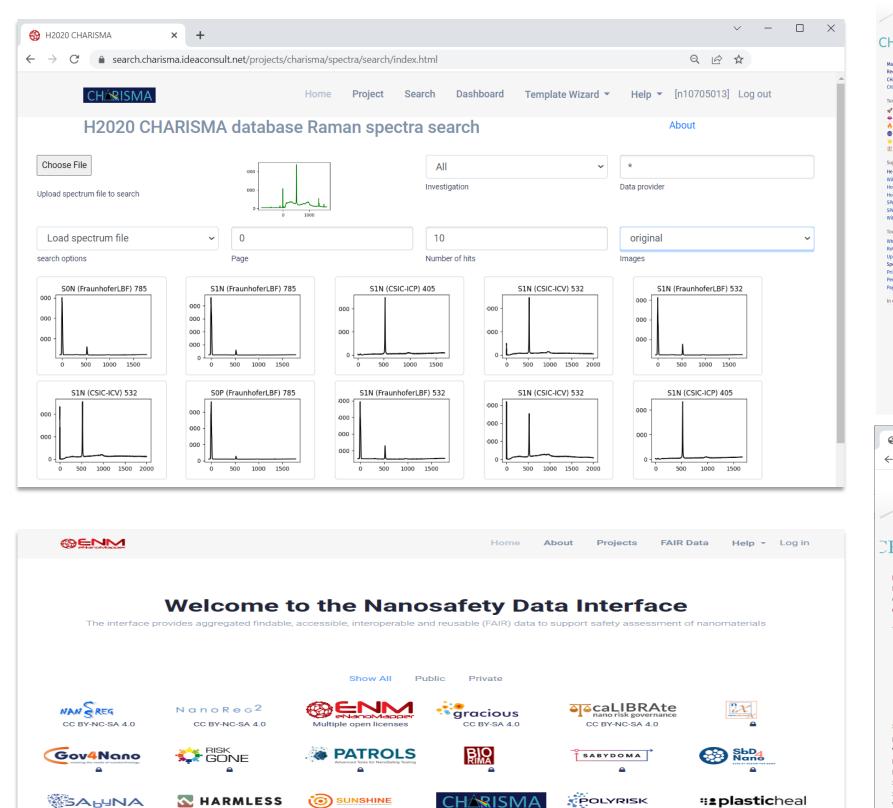


1400

Results



✓ Open source for Raman spectra harmonisation, calibration workflow Chemometric, e.g. qualitative analysis for chemical component mixtures \checkmark ramanchada2 is used as a core dependency of a FAIR Raman database, implemented as Python API with a cloud backend for storing Raman spectra and metadata in HDF5 format. The metadata query and spectra search API is compatible with eNanoMapper database and NanoSafety Data Interface [4]. \checkmark For the harmonisation of Raman spectroscopy terminology, a collaboratively edited established knowledge base at IS https://wiki.charisma.ideaconsult.net/. It is implemented with Wikibase, an extension for the MediaWiki software (https://www.mediawiki.org/), which is used by many popular wikis and, most notably, by Wikipedia.



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| rt liscussion scussions terms | | Term denotes duplicate English labels | • Evaluation • | Preferred rank | ◆ Assigned to | ◆ test discussion ^[1] | • ber of definitions ^{[2} | ♦ Synonyms ^[3] | ↔ ≥ 20 characters ^[4] | ↔ ≥ 4 words ^[5] | ↔ las a def. in English ^[6] | ↔ Non-English defs. ^[7] | + Defs. have references | ↔ Ion-English names [[] | ↔ English aliases ^[10] | ↔ on-English aliases | ♦ glish description ^[12] | + n-English descrs. ^{[12} | ¢ | + By whom | + Timestamp | By whom |
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| | Active fiber opt | ic chemical sensor | NONE | N | Jfernandez talk | | 1 | | PASS | PASS | PASS | | PASS | | | | | | 2022-04-28 19:30:00 | Idea-student talk | 2022-04-28 19:31:36 | |
| ere Iges | Advanced inver | ted mode operation | NONE | N | Antzio talk | | 1 | | PASS | PASS | PASS | | PASS | | YES | | | | 2022-04-28 16:43:29 | Idea-student talk | 2022-04-28 17:13:33 | Kerberizer talk |
| - | Airy disk | | NONE | Y | | - | 2 | | PASS | PASS | PASS | | PASS | es | YES | | | | 2022-02-10 10:54:54 | Kerberizer talk | 2022-04-17 20:51:10 | Kerberizer talk |
| s sion | Aliasing | | NONE | Y | JMTELODIZ talk | - | 1 | | PASS | PASS | PASS | | PASS | | YES | | | | 2022-04-28 19:31:47 | Idea-student talk | 2022-06-06 15:24:49 | |
| ink | Alignment | | NONE | Y | Sobr talk | 2022-04-01 11:43:30 | 1 | | PASS | PASS | PASS | | PASS | es | | | | | 2022-02-10 10:58:33 | Kerberizer talk | 2022-05-17 08:23:59 | |
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4. Jeliazkova, N et al. Nat. Nanotechnol. 16, 2021, 644–654 <u>https://doi.org/10.1038/s41565-021-00911-6</u>



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