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Towards Open, FAIR and Intelligent Raman Spectroscopy

The industrial and academic use of Raman spectroscopy grows in parallel with the need to collect, process, share and reuse digital spectroscopic data efficiently and reliably. Therefore, harmonization and standardization efforts in Raman spectroscopy are essential. In this context, we present:

a) New proposals for Raman instrument calibration and harmonisation, including samples and protocols (CWA 18133:2024 and CWA 18134:2024).

b) The open-source Python package ramanchada2, along with user-friendly, code-free downloadable and web applications, integrating existing and novel state-of-the-art algorithms for generating, reading, and processing Raman spectra, with special emphasis on calibration and algorithm benchmarking   .

c) NeXus data format adapted to Raman spectroscopy to package characterization data with metadata - including processing information- from multiple experiments and even different techniques into a single file using a harmonized structure and terminology.

d) An open source database solution that stores spectra in NeXus format with efficient metadata and spectra search, making it easier to find and compare data from different experiments.

These efforts, part of CHARISMA project (GA952921), pave the way toward FAIR (Findable, Accessible, Interoperable, and Reusable, but also For Artificial Intelligence Readable) Raman data for intelligent processing, which will benefit both private companies and open science. To foster this transformation, stakeholder's engagement and efforts coordination are crucial.

References

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