

New Approaches to Raman spectra analysis

PyRamanGUI[1, 2, 3] is a versatile tool to analyze Raman spectra, which combines state-of-the-art analysis methods like baseline correction, smoothing, cosmic spike removal, peak fitting and multivariate statistical methods like principal component analysis with the organization of Raman data in projects and the plotting of spectra. The automated evaluation of batches of Raman spectra is also available.

The projects allow to store additional information on experimental details and samples together with the data, plots and evaluated Raman spectra. The program is constructed as a graphical user interface, so no knowledge in coding is required for its use. The source code is completely written in Python and freely available (<https://gitlab.com/brehmsi/PyRamanGUI>).

In a next step we want to improve on automatic identification of Raman bands using information from databases of Raman spectra. One idea for future development is to implement a neural network that can suggest possible materials or material combinations matching an experimental Raman spectra from an unknown material.

References

- [1] GitLab repository mit dem Code: <https://gitlab.com/brehmsi/PyRamanGUI>
- [2] S. Brehm, C. Himcinschi, J. Kraus, J. Kortus, SoftwareX, 23, 101486, 2023
<https://doi.org/10.1016/j.softx.2023.101486>
- [3] Simon Brehm, Dissertation 2023 <https://nbn-resolving.org/urn:nbn:de:bsz:105-qucosa2-884021>

References

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