

# Modeling X-ray Raman scattering with XSpectra

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X-ray Raman Scattering (XRS) spectroscopy has become increasingly popular in condensed matter physics and chemistry during the last decades for probing the local atomic and electronic structure of solids, liquids or gases under complex sample environments, opening up a wealth of possibilities for *in situ* experiments. XRS bears a lot of similarities with soft x-ray absorption and electron energy loss spectroscopies, as it probes the same electronic transitions under experimental conditions where the dipole approximation remains valid, but it differs in one essential point from these techniques in that it can allow large momentum transfers and therefore induce high-order electric multipole transitions. Although N<sub>4,5</sub> edges of lanthanides and O<sub>4,5</sub> edges of actinides provide the most striking examples of such high-order transitions, non-dipole transitions can also be probed at K edges of light elements and consist predominantly of monopole or, usually to a much lesser extent, quadrupole transitions.

Modeling therefore plays a very important role when interpreting the complex *q*-dependence of XRS spectra with the purpose of extracting useful information about the local atomic or electronic structure of a material. In this talk, I will present an efficient technique designed to calculate XRS spectra at the K edge in the framework of a single-particle theory [1]. We have implemented the calculation of the XRS dynamic structure factor in the module XSpectra [2-4] of the Quantum ESPRESSO suite of codes [5] which is based on Density Functional Theory, uses pseudopotentials, a plane-wave basis set and periodic boundary conditions. The calculation is based on an efficient recursive scheme to compute the dynamic structure factor as a continued fraction without requiring the explicit calculation of high-lying unoccupied states. In this framework, multipole transitions are calculated to provide a full account of the *q*-dependence of XRS spectra.

After giving a general presentation of the method, the related approximations and practical issues, I will present the results obtained on a series of K edges recorded in lithium-bearing reference compounds, namely LiBO<sub>2</sub>, Li<sub>2</sub>CO<sub>3</sub>, Li<sub>2</sub>O, and LiF.

## References

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