Crispy: a Modern User Interface for Simulating Core-Level Spectra

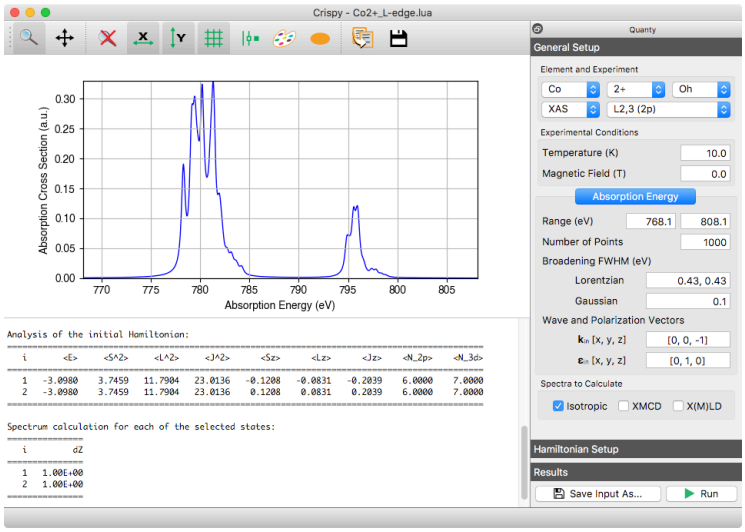
Marius Retegan, European Synchrotron Radiation Facility
marius.retegan@esrf.fr

Crispy[1] is a graphical user interface for the calculation of core-level spectra using semi-empirical multiplet theory as implemented in the Quanty[2] scripting language. Crispy provides a set of tools to generate input files, submit calculations, and plot the calculated spectra.

Following a brief introduction of the theoretical aspects, the features of the user interface will be presented in detail. With the current release, it is possible to easily perform X-ray absorption (including X-ray dichroism) and resonant inelastic X-ray scattering simulations for transition metals and lanthanides for different site symmetries of the absorbing atom. Initial support has been added for angular dependent calculations. In the case of non-centrosymmetric site symmetries, it is possible to include elaborate p-d mixing terms.

Crispy is a free and open source software, written in Python that relies on a number of additional open-source scientific libraries which are part of the Python ecosystem. The program runs on all major operating systems, and special attention was given to provide easy to use package installers for Windows and macOS operating systems in order to make the interface more accessible for non-expert users.

More information about the project, download links, and tutorials can be found on the official webpage at http://www.esrf.eu/computing/scientific/crispy.



The main window of Crispy showing the calculated XAS spectrum for Co^{2+}.

1. (1)

1. Retegan, M. *Crispy v0.4.1*. **2018**, DOI: 10.5281/zenodo.1008184.
2. Haverkort, M. W. *J. Phys. Conf. Ser.* **2016**, *712*, 012001.