Rietveld method is often used for relatively simple and routine analyses such as quantitative or lattice parameter analysis, but it was originally developed as a crystal structure refinement method and it still gives us detailed information such as atomic positions and site occupancies when used correctly. In this study, we focused on the site occupancy refinement and demonstrated how to refine it safely and more accurately.

The first thing to do is to make sure that the site occupancy you are interested in is a parameter that has a significant influence to the diffraction pattern and thus can be safely refined. If this is not the case, you could enhance its influence by selecting the right X-ray wavelength which is more sensitive to the change of that particular site occupancy. The scattering factor of an element depends on the X-ray wavelength and it changes drastically when the X-ray wavelength is close to one of the element’s absorption edges. This means that you can increase the sensitivity of your analysis by using a wavelength close to an absorption edge of a particular element whose site occupancy you want to refine.

This presentation shows how to enhance the sensitivity of your analysis by changing the X-ray wavelength. We will also demonstrate this technique using BaFe$_x$Al$_{(1-x)}$O$_{19}$. 