The supervisory board of the Kestcells Project announces the Seminar FUB-01:

# "*Extracting information from Rietveld refinement*"

***Dates***: 29.04.2013; 9:30 – 16:30.

***Place***: Helmholtz-Centre Berlin for Materials and Energy, Department Crystallography, Germany

***Summary***: Rietveld refinement allows the determination of crystal structure parameters from powder diffraction data. This seminar focussed on the extraction of reliable information from this method by selection of appropriate models, proper restraining and subsequent data analysis. Familiarity with the Rietveld method and with the basic functions of the widely used FullProf Suite was assumed, so that implementation into the refinement model could be exercised.

## *Program*

| *Time* | *Details* |
|---|---|
| *9:30 – 10:30* | *Simultaneous refinement of multiple data sets & phases, with particular emphasis on the combination of X-ray & neutron diffraction data* |
| *10:30 -11:30* | *Peak shape & asymmetry selection and their effect on the refined values of crystallographic parameters* |
| *11:30 – 12:30, 13:30 – 14:30* | *Microstructure analysis from anisotropic peak broadening: available models, necessary restraints, interpretation of the output provided by FullProf* |
| *14:30 – 15:00* | *Site occupation factors: correlation with other parameters, identification & implementation of suitable restraints* |
| *15:00 – 15:30* | *bond valence analysis* |
| *15:30 – 16:30* | *calculation of Fourier maps and their interpretation* |

## *Speaker:*

Dr. Daniel Többens, instrument scientist of the fine resolution neutron powder diffractometer at the Berlin Research Reactor BERII and instrument scientist at the diffraction beamline of the Berlin Synchrotron Radiation Source BessyII.