

**INVITED LECTURE****PROF. DR. KAY DIEDERICHS***University of Konstanz, Germany*

Kay Diederichs finished his doctorate thesis at the Faculty of Chemistry at the University of Freiburg. Since 1995 he works in Konstanz, where he is a professor of Molecular Bioinformatics at the Department of Biology, University of Konstanz. His main work is focused on structural biology and bioinformatics. He is a co-author of the XDS program package.

At the HEC24 meeting Kay will give lecture named "A better understanding of X-ray data quality indicators" that will explain the concepts behind X-ray data quality indicators, which are still not appreciated by many practicing crystallographers, are frightening for novice crystallographers, and lead to unfortunate decisions in data collection

and processing as well as refinement if not understood correctly. Warning: the talk may destroy some myths!

**A BETTER UNDERSTANDING OF X-RAY DATA QUALITY INDICATORS**

The talk first explains the concepts behind X-ray data quality indicators, which are still not appreciated by many practicing crystallographers, are frightening for novice crystallographers, and lead to unfortunate decisions in data collection and processing as well as refinement if not understood correctly. The second part of the talk will report new results that highlight the relation between accuracy and precision, by analysing simulated data that differ in

mosaicity, cell parameter variation, wavelength dispersion and beam divergence. These simulated data were used for refinement using a close-to-optimal model as starting point. The results are surprising and lead to a re-evaluation of current understanding of model and data error. Furthermore, simple guidelines for measurements with pink beam will be given.