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Abstract

X-ray absorption spectroscopy. Methods of data analysis.

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The main idea of this lecture is to overview existing methods and software packages for the analysis of X-ray absorption spectra and to describe ideas and approximations that are used in these methods. The purpose is to help participants to select appropriate software suitable for their scientific problem and to give basic knowledge required at the level of software user. In particular the influence of single electron approach, muffin-tin approximation for the potential and spin-orbit splitting on calculated X-ray absorption near edge spectra (XANES) will be described and possible range of application of such approximations will be overviewed. Then methods used for structural refinement on the basis of XANES fitting will be introduced. Finally approaches that are efficient for the analysis of big series of spectra that are based on principal component analysis will be classified.