Disorder effects in EXAFS spectra: molecular dynamics vs reverse Monte Carlo simulations

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X-ray absorption spectroscopy (XAS) is an excellent tool to probe the local environment in crystalline, nanocrystalline and disordered solids, liquids and gases in a wide range of in situ and in operando conditions. With the tremendous improvement in synchrotron radiation sources parameters, the quality of the experimental X-ray absorption spectra has increased significantly. As a result, more accurate and reliable structural information can be extracted from the extended X-ray absorption fine structure (EXAFS) located above the absorption edge of an element.

The contribution of static and thermal disorder is one of the largest challenges for the accurate determination of the atomic structure from EXAFS. Although there are a number of generally accepted approaches to solve this problem, which are widely used in the EXAFS data analysis, they often provide less accurate results when applied to outer coordination shells around the absorbing atom. In this case, the advanced techniques based on the molecular dynamics and reverse Monte Carlo simulations are known to be more appropriate [1, 2]: their strengths and weaknesses will be discussed.

References

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