

Structural properties of disordered systems: a combined Molecular Dynamics and XAS approach

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Accurate knowledge of liquid structure represents one of the challenges of modern research. In this framework, X-ray Absorption Spectroscopy (XAS) played a major role to unravel many structural aspects of liquid media. However, a reliable analysis of the XAS experimental data is a non trivial task when this technique is applied to the study of disordered systems and a very powerful approach to obtain accurate structural information on liquids is to combine XAS with Molecular Dynamics (MD) simulations. The importance of combining MD and XAS is now well recognized and allows one on the one hand to confirm the validity of the theoretical structural results and, on the other hand, to properly analyze the experimental data. In this talk examples of applications of this combined MD-XAS approach to investigate several liquid systems, such as ionic solutions and ionic liquids, will be presented. Moreover, recent results on the application of XAS to the study of chemical reactions in solution will be shown.