Structure of molecular systems and liquid metals probed by XAS and Reverse Monte Carlo

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X-ray absorption spectroscopy (XAS) is largely used to derive atom specific information on the average distribution of nearest neighbours, and beyond the pair correlations when combined with suitable data analysis strategies. In our previous studies, Reverse Monte Carlo (RMC) modelling of XAS data[1] has been applied to analyse the structure of several liquid metals under extreme conditions and to address important issues, such as the extent of local icosahedral ordering[2] or the occurrence of pressure induced structural transitions[3].

Within this contribution, we present recent developments of the RMC-GNXAS[4] approach (and code) and newly added features including multi-atomic and multiple-edge refinements. A few applications of RMC to XAS and diffraction data of several gas-phase molecules and binary alloys will be discussed.

RMC-GNXAS has been used for the analysis of x-ray absorption spectroscopy (XAS) multiple-edge data sets for six gas phase molecular systems (SnI_2, CdI_2, BBr_3, GaI_3, $GeBr_4$, GeI_4)[5]. Sets of thousands of molecular replicas were involved in the simultaneous refinement of XAS data and electron diffraction results. The validation of this approach on simple molecular systems is particularly relevant as a basis for the method application to more complex and extended systems including metal-organic complexes, biomolecules, or nanocrystalline systems.

For liquid Sn-based metallic binary alloys[6], the combination of XAS and RMC allowed us to obtain three-dimensional models of the local structure compatible with present experimental evidence overcoming some limitations of standard approaches.

References:

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