Analysis of EXAFS data beyond conventional approach

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Current strategies for the analysis of EXAFS data are usually based on a peak-fitting analysis in which information is limited to average quantities like bond lengths and vibrational amplitudes, often assuming a Gaussian distribution of distances. This approach is certainly justified for molecules and for ordered condensed matter. However, even in these cases, the problem of defining suitable model functions may be particularly severe. The intrinsic limitations of the peak-fitting technique may be overcome by using model-independent methods in which the shapes of the distribution functions are not defined "a-priori". Two different data-driven methods are presented: Reverse Monte Carlo and Sparse Modeling.

Reverse Monte Carlo (RMC) [1] is an inverse modelling technique for producing three-dimensional structural models from experimental data. The combined refinement of XAS and diffraction data allowed us to investigate gas phase molecules [2], elemental liquid metals [3] and alloys [4], for which estimates of the fraction of nearly-icosahedral configurations and bond angle distributions were obtained, both in the liquid and undercooled liquid phases.

In Sparse Modeling we solve a system of linear equations with the additional requirement that the solution vector is sparse, using a least absolute shrinkage and selection operator (LASSO). In condensed systems, we can approximate the radial distribution function as a sparse vector and therefore solve the EXAFS equation [5], obtaining structural information of the system.

References:

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