

# Statistical view on core-level spectra of liquids

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Rather than a single geometry, the atomistic structure of liquid systems is described by a collection of possible configurations, each assigned with a probabilistic weight for occurrence [1]. This fact means that all properties derived from atomistic configurations are averages over the corresponding statistical ensemble. Most notably for spectroscopists, X-ray spectra from liquids are not an exception to this principle.

In this contribution we will discuss the consequences of this idea, using our recently established line of thought [2-4] as an example. We start with the fundamental difference between a gas-phase and a liquid system, and then proceed with the idea of ensemble averages as the only obtainable experimental result.

What follows is a method of analyzing statistical simulations for structural interpretation of the core-level spectra. The protocol [2-3] relies on a a-posteriori analysis of a simulation for the ensemble averaged core-level spectrum to establish a statistical link between structural information and spectral regions of interest. Here, the role of core-level spectroscopy is fundamental: as the 1s orbital is local, each individual transition occurs locally, which allows for connecting the behaviour of averaged spectra to atomistically local structural parameters.

Last, we will quickly refer our current view of what this means for interpretation of the X-ray spectra of liquid water in ambient conditions [4].

## References

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