Information theory tools to study liquid structure

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The study of the structure of disordered phases is inherently complicated. Short range order of liquids is encoded in a six-fold Probability Distribution Function (PDF) which describes the most probable relative position and orientation of two molecules at a given distance. For plastic phases, the degree of complexity is slightly lower since, at least, the molecular position is fixed by a long range ordered crystalline lattice. But still, the relative position of molecules with respect to this lattice, and the relative position of two molecules, i.e. the short range order, must be again encoded in a multi-dimensional PDF.

The aforementioned PDFs, or at least their 2D and 3D projections, can be investigated to provide an exact description of molecular ordering at a given distance. But many of the times we are not interested to investigate the structure at such a level of specificity. That's why we have applied the tools based on Information Theory, such as Shannon entropy, mutual information, or the Kullback-Leibler divergence to the description of disordered phases. These tools allow us to obtain a global description of the structure of disordered phases. Moreover, these calculations guide us to focus on the research of some features of the structure that might be worth to investigate with more detail.

REFERENCES

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FIGURES

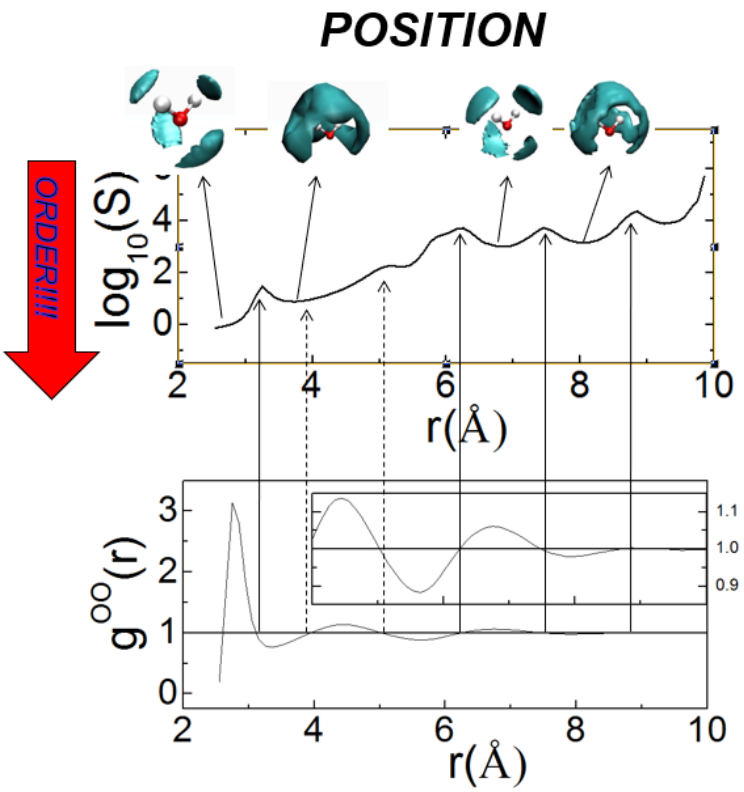

Figure 1: Oxygen - oxygen radial distribution function of water in the lower panel. In the upper panel Shannon entropy related to the positional molecular ordering, together with the 3D-density maps associated to molecular positions.