Seminario

Viernes 12 de abril de 2024 – 11:30 h

Sala de Tesis (Antigua Capilla)

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Structure determination by simultaneous fitting to multiple experimental data sets

Different experimental probes are sensitive to different aspects of the structure and interactions in a sample. Thus, it becomes essential to combine information from as many experimental probes as possible when determining structural parameters of complex systems - and to also test hypotheses and range of validity. I will illustrate with regular Reverse Monte Carlo (RMC) applied to X-ray and neutron diffraction data on liquid water combined with infrared Raman to determine structure and test hypotheses on hydrogen-bond connectivity in liquid water [1]. In this case the time required for property evaluation was short enough to allow atomistic moves. However, evaluating spectroscopic properties from a model is too time-consuming to allow 108-109 MC steps.

Here we use our SpecSwap-RMC method [2] to extract structural data by instead focusing on property moves based on a large library of precomputed properties from a broad selection of possibly relevant structural models. I will illustrate by application to EXAFS and diffraction data on liquid water [3], XAS, XES and the O-O RDF of liquid water [4]. In the latter case, for XES, I will also describe the genetic algorithm introduced to connect spectra computed at different time-steps along the core-hole-induced trajectories [5]. Finally, I will discuss ongoing work using EXAFS on Argon as probe of low-density-like local environments in water.

[1] Leetmaa *et al., J. Chem. Phys.* (2008) 129, 084502.

[2] Leetmaa *et al., J. Phys.: Cond. Mat.* (2010) 22, 135001.

[3] Wikfeldt *et al., J. Chem. Phys*. (2010) 132, 104513.

[4] Pettersson and Takahashi, *J. Non-Crystalline Solids: X*, (2022) 14, 10087.

[5] Pettersson and Takahashi, *Theor. Chem. Acc*. (2021) 140, 162.