Modelling NMR Properties of Oxide Glasses with Machine Learning

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Solid-State NMR has become an essential spectroscopy for the elucidation of the glass structure. With recent advances in DFT computations, NMR can now be combined with Molecular Dynamics (MD) simulations to help interpret the experimental data [1] because the spectral broadening associated with the structural disorder of glass that often limits their detailed interpretation of NMR spectra. However, such calculations are severely limited in system size by the high- computational cost of DFT computations.

In recent years, machine learning (ML) approaches have emerged as a powerful method for accelerating MD and computing materials properties with an accuracy close to that of DFT methods. [2] In solid state NMR, few approaches have been recently proposed that can be applied to oxide glasses [3] which are complex materials with structural features that are still debated. We describe here an approach based on the concept of atomic-centered descriptors[4] (such as SOAP) combined with Kernel Ridge Regression (KRR) or Artificial Neural Network (ANN) techniques. This enables the prediction of NMR properties for structural models of thousands of atoms in a few seconds. Its combination with Monte Carlo simulations methodologies combining MD, NMR and neutron data will be illustrated through several applications to simple borate and silicate glasses.

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[3] Chaker et al. *NMR shifts in aluminosilicate glasses via machine learning*. Phys. Chem. Chem. Phys. (**2019**) 21, 21709
[4] A. P. Bartók, et al. *On representing chemical environments*, Phys. Rev. B, 87.18: 184115 (**2013**).