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Solid-State NMR has now become a key spectroscopy in numerous fields of material sciences. The local environment of each atom is characterized by a NMR fingerprint that can be acquired independently of the crystalline, disordered or vitreous form of the studied material. With recent advances in DFT computations, NMR can now be combined with Molecular Dynamics (MD) simulations to help the interpretation of experimental data. However, such calculations are severely limited in system size by the high- computational cost of DFT computations.

In the last years, machine learning (ML) approaches have emerged as powerful mehods for accelerating MD and computing materials properties with an accuracy and an efficiency that are close to that of DFT methods and classical MD, respectively. In the specific field of solid state NMR, few approaches have been recently proposed that can be applied to oxide glasses which are complex materials which structural features that are still debated. We describe here an approach based on the concept of atomic-centered descriptors (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. An optimal scheme based on the Least-Square Support Vector Regression algorithm will be presented with applications to simple borate and silicate glasses.

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