



HAL
open science

Modelling NMR spectroscopy of oxide glasses with machine learning

Thibault Charpentier

► **To cite this version:**

Thibault Charpentier. Modelling NMR spectroscopy of oxide glasses with machine learning. 1ères Journées GDR IAMAT, May 2022, Paris, France. cea-03687152

HAL Id: cea-03687152

<https://cea.hal.science/cea-03687152>

Submitted on 3 Jun 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Modelling NMR Spectroscopy of Oxide Glasses with Machine Learning

Thibault Charpentier

¹Université Paris-Saclay, CEA, CNRS, NIMBE, CEA Paris-Saclay, Gif-sur-Yvette, 91191, France,
thibault.charpentier@cea.fr

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 methods 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.

sciencesconf.org:gdr-iamat:408065