My research project is focused on glass science and on developing new simulation methods to improve the description of amorphous structures and the predictive power of simulations.

Nowadays, NMR (and in particular solid state NMR) has established itself as the most advanced spectroscopy method allowing for reliable structural investigations in amorphous systems. This is mainly due to its sensitive and isotopically selective character in probing the local environment of atoms and so it can provide detailed structural information. The interpretation of NMR spectra, based on computational methods, has relied, so far, on DFT calculations, in particular since the breakthrough development of the gauge-including projector augmented wave approach (GIPAW). Even if this method has lead to impressive results, it suffers the great limitations of high computational cost. A new challenging method that can provide ab-intio accuracy with reduced computational cost in the NMR interpretation is the application of machine learning (ML) techniques.

Machine learning methods are mainly based on artificial neural network (NN), which are biology-inspired algorithms that provide an accurate tool for the representation of arbitrary functions. The structure of a neural network is made by layers of node (or neuron) linked together by weighted functions. In particular, there are an input layer, an output layer and, in between, a variable number of hidden layers, each one containing a certain number of neurons linked with every node of the previous and subsequent layer. The main idea of ML is to train the machine with a huge amount of accurate input-output data (training set) as the algorithms can find the best parameters for every neural link to reproduce the known output minimizing a cost function. The number of connection between neuron is normally very high and allow to obtain a very flexible fit of accurate data. Once this method is trained and tested, it can be applied to unknown systems.

Input data are often referred to as descriptors as they have to be suitable for the description of the system. For the NMR parameters prediction, a set of descriptor that represents the local environment of each atom have to be constructed, as NMR is a local (atom-centered) spectroscopy. There are many other factor that have to be optimized for a good machine learning, such as the number of hidden layers and nodes and the kind of weighted function that relates neurons of different layers.

Machine learning techniques, in material science, can be applied to a very wide range of property predictions (elastic constants, mechanical properties, chemical durability, etc …) as it is a very powerful and flexible method.

A very challenging, but possibly revolutionary, application of ML algorithms is the generation of ML-Force Fields. In this case, the network is trained to reproduce forces between atoms with almost ab-initio accuracy, but with classical MD effort.