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Machine learning implementation for predicting crystal structures of materials

We intend to study the crystallization of molecular substances using machine learning techniques. Direct observation of crystal symmetries in simulations is often quite challenging. The crystallization proceeds through a nucleation mechanism that may involve nuclei of considerable size over long periods of time. In addition, the final crystal can be influenced by the boundary conditions and the initial state. On the other hand, it is known that it is the short-range interactions between molecules that determine the long-range crystalline structure of the compounds. Simulations of small molecular clusters by QM/MM (quantum mechanics/molecular mechanics) techniques provide a wide set of molecular descriptors such as the free energy of cluster formation, the Steinhardt parameters and atom-atom distance matrices. The crystalline structure is a well defined categorical set determined by the crystal symmetry that consists of 230 space groups. This framework is well suited for study using neural networks where the multiple input array produces one of a number of possible outputs. We propose to combine expertise on cluster simulations developed in the group with the neural network techniques to predict crystal symmetries of molecular compounds. An outcome of the project is an expert system that takes as an input an array of structural descriptors and provides as an output a tentative crystal structure of the molecular compound.

The project will be done in collaboration with scientists in the Chemical Engineering Department at Western, where they study crystallization of pharmaceuticals by experimental methods.
Overall, the student involved in the project is expected to have some skills in computing or being able to progress rapidly (in approximately a month) in building the computational skills.

References

See the 4th year undergraduate thesis: `` The Implementation of Machine Learning to Predict the Solubility of Simple Organic Molecules'', Ryan O'Dwyer (2020).