

*Crystallography, artificial intelligence and the interaction between atoms*

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The discovery of new materials plays a key role for developing the different kind of technologies. For example, for producing energy, reducing air pollution, or developing new detectors for medical applications. Sometimes new materials are discovered by trial and error experiments done by researchers that have a large experience in solid state chemistry, who had "learned" key features for the synthesis of materials. Another way for discovering new materials is to understand the behavior of materials on the atomic level. For example, through experiments with X-ray, neutron and electron diffraction and some spectroscopic analysis. The interpretation of these experiments, however, requires a good idea about the electronic structure of the material. Nowadays, this information can be obtained through empirical models describing the interaction between atoms, or using quantum mechanics, which provides very precise information about the electronic and atomic properties, whereas the empirical models give only a rough first approximation to them. To use a model based on quantum mechanics needs a huge capability of computation. Although nowadays computers can perform hundreds of PFLOP/s, the number of atoms in a system that can be analyzed with quantum mechanics is confined to some thousands. This also limits the analysis of the time evolution of atoms to the range of picoseconds, whereas the information obtained in experiments occurs in nanoseconds or larger times. The empirical models for the interaction between atoms can analyze systems having several orders of magnitude more atoms than those analyzed with quantum mechanics, because they use functions for describing this interaction. During the last decade, it has been shown the possibility to combine the techniques of artificial intelligence, and quantum mechanics to generate multidimensional functions that describe the interaction between atoms with the precision obtained with quantum mechanics. In this case, a set of quantum mechanical calculations of the system are used to train an artificial neural network for "learning" the interaction between atoms; the network generates a function, having hundreds or thousands of parameters, that describes this interaction. This function can be used to predict the behavior of systems with the same type of atoms but with a larger number of them; it is also used to perform molecular dynamic calculations for times of nanoseconds or larger. This methodology requires to find important features of the atomic arrangement for the input layer of the artificial neural network that be related with the potential energy of the system. Until now, the features used to describe the system are based on the traditional models used to generate the empirical potentials describing the interaction between atoms, which are basically related to the atom properties and their interaction to build molecules. In the present work, we show that crystallographic information of the system can be used to generate the features required by the artificial neural network. We show that the crystallographic sites that describe the atomic distribution in a solid are more important for generating these features than the atomic properties of the atoms that occupy them.

**Keywords:** [quantum mechanics](#), [artificial neural network](#), [interaction between atoms](#)