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Fast and reliable crystal structure prediction using random search algorithms and machine learning interatomic potentials

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The position that ions occupy in the unit cell of a crystal and in the periodic table of elements, fully determines the physical, chemical and functional properties of materials. Through diffraction experiments, such as X-ray and neutron scattering, it is possible to determine the crystal structure of a material. However, when such experiments are difficult to conduct (e.g. requiring high-pressure conditions) and in situations in which rational guides are required to avoid expensive and time-consuming trial-error searches (e.g. design of new drugs), conducting initial crystal structure prediction (CSP) studies may provide useful insights. This is a formidable complicated problem, since stable and meta-stable phases are related with minima in the energy hyper-surface of the configuration space, and to explore this surface is a tremendously complicated task [1]. Different methodologies of CSP have been developed and proven useful in various situations [2]. Here we present PyMCSP [3] (Python and Machine Learning methods implementation for Crystal Structure Prediction). The program uses random search methodologies to look for the energy minima, by using the PyXtal library [4] to generate different phases with different symmetries compatible with the stoichiometry of the material. Afterwards, the structures are relaxed using machine learning interatomic potentials with M3GNet [5], and ranked according to their energy. By proceeding in this manner, we avoid the use of computationally intensive first-principles calculations (e.g. density functional theory, DFT) and supercomputer facilities so that full CSP analysis can be carried out in very short timeframes using only a laptop. It is possible to determine a theoretical diffractogram of the resulting phases and compare it to those obtained experimentally, in order to assist with space group identification. The reliability of the results has been tested in different materials, for example obtaining some of the meta-stable phases of the polymorphic materials BN or Ag3SBr.

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Primary author: BENÍTEZ COLOMINAS, Pol (Universitat Politècnica de Catalunya)

Co-authors: Dr CAZORLA, Claudio (Universitat Politècnica de Catalunya); Prof. SAUCEDO, Edgardo (Universitat Politècnica de Catalunya)

Presenter: BENÍTEZ COLOMINAS, Pol (Universitat Politècnica de Catalunya)

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