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A machine learning-based web platform for crystal system classification: CrystalMELA

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A new machine learning (ML) based web platform, named CrystalMELA (Crystallographic MachinE LeArning), for crystal system classification, has been developed.

In the current version, the tool is able to run three different and complementary ML models: a Convolutional Neural Network (CNN), a Random Forest (RF) and an Extremely randomized trees (ExRT). The models have been trained on theoretical powder diffraction patterns of more than 280,000 crystal structures of inorganic, organic, organo-metallic compounds and minerals as collected in the POW_COD database[1]. A 70% of classification accuracy was achieved, improved to 90% if the top-2 accuracy is considered.

CrystalMela is free availability at <http://www.ba.ic.cnr.it/softwareic/crystalmela/>, its home web page is shown in Figure 1. The classification options in CrystalMELA platform are designed to be powerful and easy to use, supported by a user friendly graphic interface. Their main aspects and some examples of applications to real cases, will be presented.

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