ARL/Master Thesis

in the group of *Theory of Magnetic Materials* (FB11)

TECHNISCHE UNIVERSITÄT DARMSTADT

Deep Learning Design of Magnetic Materials

Magnetic materials have a wide spectrum of applications as energy materials. Thus the design of new magnetic material is of great importance. With the development of machine learning in particular deep learning techniques, inverse design to automatically design functional materials has been established.

Recently, we have successfully developed a method to transform the known crystal structures into the crystal graphs (cf. Fig. 1), and implemented a generative adversarial network model to predict novel crystal structures, using more than 52,000 materials in Materials Project as the training set. In this project, we will endeavour to incorporate the available magnetization data into the deep learning model so that stable magnetic materials will be predicted, focusing on building a convolutional neural network model on the magnetization.

For the motivated candidates, expertise will be gained on GPU-computation, coding with Python, and possible experience on sophisticated density functional theory calculations, valuable for both future PhD studies and industrial positions.

Please write Prof. Hongbin Zhang (Email: hongbin.zhang@tu-darmstadt.de) if you are interested.

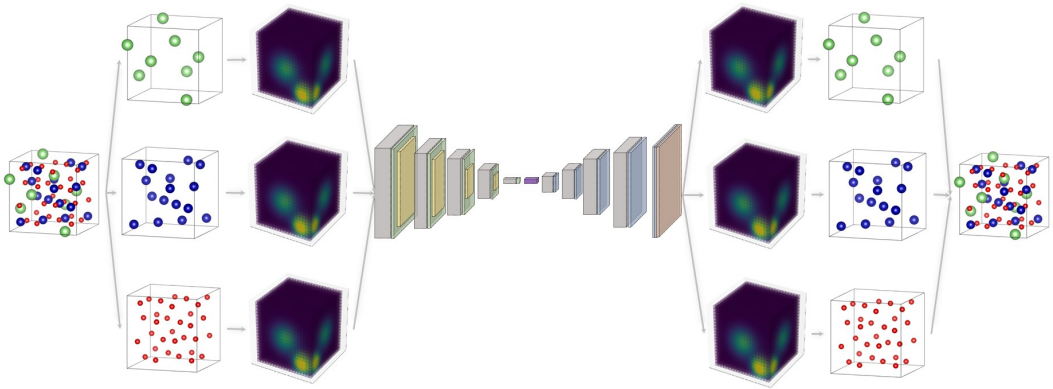

FIG. 1: Encoding and decoding of the crystal structures