ARL/Master Thesis

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

TECHNISCHE UNIVERSITÄT DARMSTADT

Generative diffusion model for crystal structures

The discovery of new inorganic materials with desirable properties is a critical but challenging task in materials science. Traditional methods of materials discovery, which rely heavily on experimental trial-and-error or computationally expensive simulations, are often time- and resource-costly. Moreover, the vastness of the chemical space makes it difficult to explore and identify promising new materials efficiently. Thus, there is a need for innovative tools that can accelerate the discovery and employment of novel materials by efficiently navigating this vast space.

In this project, we are going to focus on establishing a methodology to leverage advanced machine learning techniques, particularly deep generative models, to predict novel inorganic material compositions. The model will be trained on a large dataset of computational inorganic materials, learning the underlying distribution and optimizing the relevant physical properties in the properly constructed latent space. Once trained, the model can propose new, valid inorganic compositions that are likely to exhibit desirable properties.

For the motivated candidates, expertise will be gained in the generative diffusion model as specified in https://arxiv.org/abs/2312.03687, and coding with Python valuable for both future PhD studies and industrial positions.

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

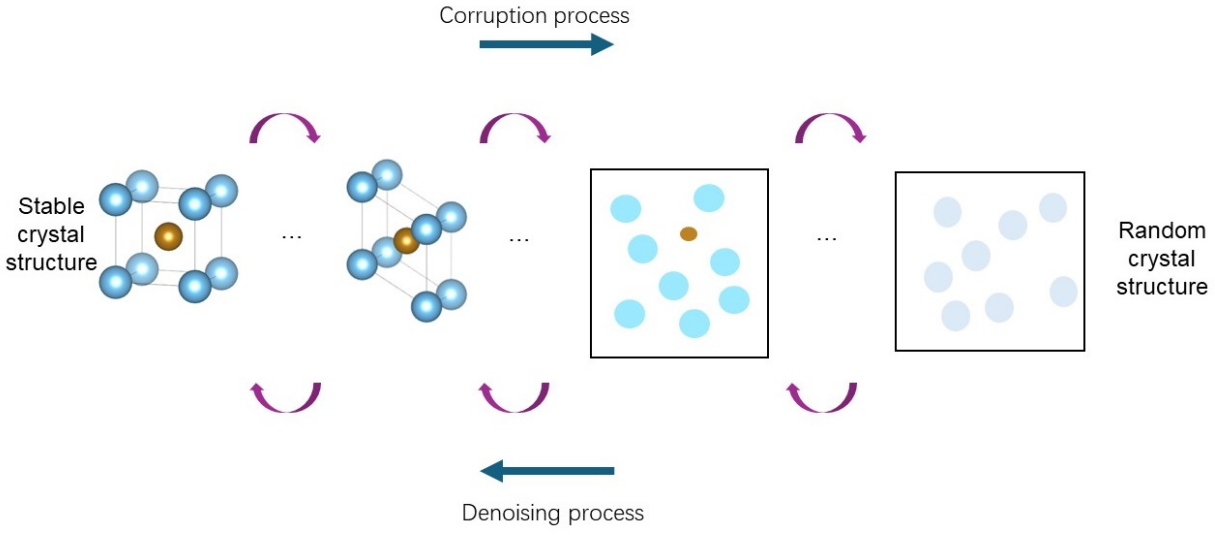

Figure 1: Generative diffusion model for crystal structure