How Foundation Models for Atomistic Modelling are Changing Materials Discovery

Johannes Margraf [1,†]

[1]Universität Bayreuth, Germany

† corresponding author's email: Johannes.Margraf@uni-bayreuth.de

The design and discovery of new materials from first principles has been a tantalizing prospect for computational chemistry for the past decades. Realizing this promise has been highly challenging due to several factors, including the vastness of chemical space, and the discrepancy between idealized crystal structures and real (potentially disordered) materials. In this context, machine learning interatomic potentials (MLIPs) have become an important tool, as they allow a more realistic description of materials due to their high computational efficiency. Until recently, MLIPs had to be developed from scratch for each class of materials, however, which is impractical for exploring large composition spaces. This has changed with the emergence of foundation models for atomistic materials chemistry, which are pre-trained for materials across the periodic table. In this talk, I will discuss how these foundation models are changing computational materials discovery, focusing on their potential for structure prediction in large composition spaces. We will also consider remaining limitations of the models and computational materials discovery more generally. For the former, we will discuss the need for electrostatics-aware and non-local models, for the latter we will discuss the role of crystallographic disorder when predicting new materials.