

Machine learning interatomic potential for metamorphic minerals

Xin Zhong

Institut für Geologische Wissenschaften, Freie Universität Berlin, Berlin 12249, Germany

The stable pressure-temperature (P-T) ranges of metamorphic minerals are crucial for the reconstruction of geological history. Conventionally, phase diagrams were constructed using thermodynamic databases fitted to experimental measurements of e.g. heat capacity, elasticity, and volume. Kinetic processes such as phase transition and chemical diffusion cannot be directly accessed without knowing the corresponding parameters such as reaction energy barrier and diffusivity. In this project, we aim at developing a suite of machine learning interatomic potential with state-of-the-art techniques on Mg-Al-Si-O system to predict phase stability at high P-T conditions. Moreover, kinetic process such as chemical diffusion will be investigated and compare to experimental observation to better understand the diffusion mechanism of minerals within the Earth's interior.