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Internal Webinar

Data driven insights into crystal structure preference in ternary compounds

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The phonon band structures of any system reveals its nature on the potential energy surface. Studies have shown that an instability can lead the unstable structure to a stable one by a normal mode displacement of the atoms in the unit cell. In our work, we have shown that these soft phonon modes are linked by a 1/q* criterion which encodes the systems preference to form a lower symmetric stable phase [1]. We study this phenomenon with a close look at Peierls and charge density wave phases in quasi-1D materials. In a later work, we show that encoding the information of symmetry of these materials systems gives rise to a novel group-subgroup machine learning methodology [2]. We show that models containing the information about a subgroup and minimal information about the group predict properties of the group better than models with information only about the latter. We show the Barnighausen tree for frieze groups which enables symmetry based analysis for our modelling.

In this talk, I will present our previous ideas in the 3 dimensional context to predict possible stable structures from unstable structures. The 1/q* criterion indicates the size of the stable unit cell and the normal mode leading to it. Group theoretical analysis also shows how two space groups are linked in the potential energy surface. High-throughput methods guarantee a better success rate for finding new materials with desirable properties. I will present our new dataset which contains previously unknown stable materials and new structures from our symmetry analysis.

References:

[1] Prakriti Kayastha and Raghunathan Ramakrishnan, Journal of Chemical Physics 154, 061102 (2021)
[2] Prakriti Kayastha and Raghunathan Ramakrishnan, in press, Machine Learning: Science and Technology

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