Rapid Mechanical Property Prediction using Wyckoff Set Regression for Scalable Materials Exploration

Timothy H. LEES (Linköping University, Sweden),
Abhijith S. PARACKAL (Linköping University, Sweden),
Florian TRYBEL (Linköping University, Sweden),
Rickard ARMIENTO (Linköping University, Sweden)

Abstract

Recent advances in machine learning have significantly accelerated materials discovery. Despite these advances, the space of all possible crystal structures and their properties is enormous, and full exploration is computationally infeasible. Exploring the combinatorial space of Wyckoff positions, capturing symmetrically inequivalent atomic positions, is a more tractable problem. The GPU-optimized transformer-based WREN (Wyckoff REpresentation regressioN) framework can be used to efficiently navigate this space. WREN has demonstrated to be highly effective in rapidly relating symmetry to formation energies on vast scales [1]. We extend its application by predicting the essential mechanical properties of bulk and shear modulus. These are necessary quantities to understand a materials behaviour and stability under high pressure. As WREN's descriptor is independent of atomic positions, this not only enables property prediction without realizing crystal structures but opens up the tantalizing prospects to rapidly screen phase competition at high pressure at an unpresented scale. I will present recent methodological developments and compare predictions with experiments, ab-initio and other machine learning approaches.

[1] Parackal, A.S., Trybel, F., Faber, F.A. and Armiento, R. (2026) *Screening 39 billion protostructures for materials discovery*. arXiv preprint arXiv:2601.21393. Available at: https://arxiv.org/abs/2601.21393 (Accessed: 29 April 2026).