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GRACE universal interatomic potential for materials discovery and design

Tuesday 27 May 2025 13:50 (30 minutes)

Universal interatomic potentials parameterize the interactions between all chemical elements in the periodic table simultaneously. In my talk I will introduce the Graph Atomic Cluster Expansion (GRACE). GRACE builds on a complete set of graph basis functions and can be viewed to generalize equivariant message passing neural networks and other machine learning interatomic potentials. I will then discuss the parameterization of a GRACE foundation model across the periodic table and compare the performance of GRACE foundation model to element-specific potentials.

The ability to simulate thousands or millions of atoms with complex chemistries for extended time scales opens completely new routes for materials discovery and design. I will demonstrate usage scenarios for widely different materials. Finally, I will discuss limitations of current foundation models and suggest steps to overcome these.

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