Foundational Graph Atomic Cluster Expansion: Bridging Quantum Mechanics and Materials Development

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Technological innovation and progress rely increasingly on the accelerated discovery, development and reliable deployment of advanced materials. However, atomistic thermodynamic and kinetic simulations have traditionally been constrained by the steep computational cost of first-principles methods and inherent simplifying approximations, limiting studies to small systems and simplified chemistries. The advent of foundational potentials in Materials Science, particularly universal Machine Learning Interatomic Potentials (MLIPs), is rapidly overcoming these limitations.

This presentation introduces the Graph Atomic Cluster Expansion (GRACE), a beyond message passing equivariant basis expansion that builds on a complete and efficient description of atomic interactions. Crucially, GRACE overcomes the fundamental scaling limits of traditional atomistic modeling. By employing efficient graph-based recursion, it circumvents the combinatorial explosion typically associated with chemical complexity in multi-component systems. Concurrently, its semi-local representation ensures linear scaling with system size, enabling accurate simulations of extended defects. I will demonstrate how GRACE unifies leading MLIP methodologies and facilitates robust thermodynamic and kinetic predictions for complex solids and advanced alloys.

Furthermore, I will address the incorporation of complex physical phenomena, such as dynamic charge transfer and magnetism. Finally, I will detail how GRACE guides the development of comprehensive first-principles databases by leveraging uncertainty quantification and maximum entropy sampling of atomic configuration space.

Ultimately, by bridging the gap between quantum-level accuracy and macroscopic materials performance, foundational frameworks like GRACE are poised to drastically reduce the time and resources required for materials development and deployment.