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Ab Initio Computations and Data-Driven Insights for Material Discovery and Superconductors

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Topics

Computations and new theoretical aspects

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Abstract

Through the combination of high-throughput ab initio computations and machine-learning techniques, we are building one of the largest databases of crystalline structures in the world, with over five million structures computed using density functional theory (DFT). Of these, more than 144 thousands are identified as thermodynamically stable, which makes it the largest convex-hull publicly available. The dataset aims to be chemically general while remaining restricted to crystalline solids. Candidate structures are first screened using machine-learning universal potentials, with final energies and structures refined through DFT+U following Materials Project methodology.

This extensive dataset not only serves as a foundation for novel material discovery and design, but also allows us to define and explore new data-driven descriptors. Among others, we can define the concept of nobility (chemical inertness) as a graph property in the convex-hull. High potential properties can also be investigated in this vast material space. For example, superconductivity has been investigated within the Eliashberg framework showing the limits to what can be achieved within the conventional mechanism. Explorations of similarity-driven search are also undergoing to uncover new unconventional superconductors. Material design, where a conjonction of several unrelated properties is desired, is also a important application of the dataset. In this talk, we will share early insights from our ongoing research and discuss prospective directions that this flexible and evolving framework may lead to.