

Accelerated Workflow for Antiperovskite-based Solid State Electrolytes



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Invited for this month's cover picture is the group of Prof. Ivano E. Castelli. The cover picture shows a battery unfolding in its main components and the charge density, which is used to accelerate the estimation of the ionic mobility of the solid-state electrolyte. Read the full text of the Research Article at 10.1002/batt.202300041.

What is the most significant result of this study?

The development of new battery technologies and materials is necessary to accelerate the transition to a sustainable future. In this work, we establish a new protocol to accelerate the estimation of thermodynamic and kinetic properties. The protocol combines quantum mechanical simulations, in the framework of Density Functional Theory, and surrogate models, based on calculated charge density. This approach is applied to discover new solid-state electrolytes for all-solid-state batteries. Although demonstrated for the antiperovskite class of materials, the protocol is general and can be used for many other structures.

This work has two main outcomes. From the technical side, it defines a new approach to accelerate time-consuming calculations, needed to estimate the kinetic properties, which are a descriptor for the ionic mobility. From the materials side, it paves the way for studies on new classes of materials where positive and negative ions are swapped compared to the conventional materials, such as antiperovskites, which are charge inverted from perovskites. These "inverted crystals" have higher ion mobility, but also lower stability. The inverted crystal class is often uncharted territory and one of the main challenges is their synthesis and use in devices.

