Cover Profile
doi.org/10.1002/batt.202000101

Chemistry Europe
European Chemical Societies Publishing

Autonomous Discovery of Materials for Intercalation Electrodes

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EMAGIC BATTERY COMMUNITY
AiMade
Autonomous Materials Discovery

Invited for this month's cover picture is the Section for Atomic Scale Materials Modelling led by Prof. Tejs Vegge at the Department of Energy Conversion and Storage, Technical University of Denmark. The cover picture illustrates an autonomous workflow, implemented in the framework of Density Functional Theory, designed to automatically calculate crucial properties for battery intercalation electrodes, including thermodynamic and mechanical stability, open circuit voltages (OCV), as well as kinetic barriers for the ionic transport. Applied here to identify cathode materials for Mg-ion batteries, this workflow enables an accelerated discovery of intercalation battery electrodes. Read the full text of the Article at 10.1002/batt.201900152.

What aspects of this project do you find most exciting?

Accelerating the discovery of novel materials is of key importance for many battery applications and devices. With this work, we aim to automatize and accelerate not only the calculations of thermodynamic properties but also of the kinetic properties, such as diffusion barriers, which are usually tedious and very expensive to estimate. We have thus implemented a fully autonomous workflow, which can identify intercalation electrode materials for batteries based on simple, but accurate descriptors, and existing structures from databases like the ICSD. The dataset generated can also enable the use of advanced statistical tools to provide a more accurate explanation of the relation between a crystal structure and its kinetic properties.

What was the inspiration for this cover design?

We imagine our computational workflow as a production line, where materials are autonomously calculated and analysed for multiple target properties. The materials, which fulfil the design criteria, are then sent for experimental validation or additional calculations, while the others are discarded.

How would you describe to the lay person the most significant result of this study?

We use computational methods in the form of Density Functional Theory, to accelerate the discovery of new battery materials, as supercomputers are able to calculate properties and identify optimal candidate materials in a fraction of the time needed by experiments to measure them. Even further, by managing all the different steps of the calculations autonomously, this workflow not only accelerates the discovery process with a minimal input from the user, but also enables the user to track every step digitally making the results fully reproducible.