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Rapid Design of Materials for Energy Applications: Methods and Data Automation Tools

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Abstract:

Design of new functional materials relying on transport phenomena is complicated by the highly nonlinear sensitivity of conductivity to structural and composition changes. This makes brute-force computational screening impossible and requires the development of descriptors and efficient approximations to narrow down the space of possibilities. I will briefly present our recent efforts on developing practical methods and data-driven approaches for the discovery and design of materials for electrochemical energy storage. In each case there is a need to automate computational tools, organize and analyze the data, and preserve full record of data flow for reproducibility, while allowing for data sharing. The resulting workflows and data formats are heterogeneous and an automation platform is needed that is flexible enough to cover the common requirements and to leave the API interfaces open for implementation of specific scientific plug-ins by the users. The necessary features include tight coupling of data capture with automation, connecting computational engines in a high-level working environment, recording complete provenance information, and organizing data in an efficiently query-able form. Finally, data science tools are also needed for analyzing transport data, extracting and validating trends, to be used in iterative screening. I will highlight our current efforts to implement an open-source AiiDA platform aimed at satisfying these requirements.