Towards an accelerated design of energy materials

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The development of new energy technologies, essential for transitioning to a sustainable future, relies on the discovery of new materials. Over the past decades, materials simulations have significantly accelerated the discovery process, complementing experimental approaches. These simulations offer unique insights into the fundamental mechanisms that drive material behavior. Additionally, they can predict material properties and elucidate the relationship between atomic structures and their properties, thereby enabling a rational design of materials with specific characteristics. Despite their success, the discovery process has traditionally been slow, requiring iterative cycles between theoretical predictions and experimental verifications until optimal materials are identified, synthesized, and tested in real devices. This paradigm has recently been broken by the creation of Materials Acceleration Platforms (MAPs), where AI-orchestrated collaboration between AI-accelerated materials simulations and self-driving laboratories enables closed-loop materials discovery.

In my lecture, I will first discuss the development of a technology-agnostic, autonomous, and standardized modelling framework and its integration into a MAP. The foundation of this infrastructure is a dynamic workflow management system capable of orchestrating calculations of thermodynamic and kinetic properties, which play a fundamental role for many energy technologies. Within this framework, we have established the first autonomous workflow to discover new electrodes and solid-state electrolytes for the batteries of the future. Beyond batteries, this technology-agnostic workflow can be applied to discover new materials for a wide range of next-generation energy technologies, from fuel cells to photovoltaics. While workflows are commonly used for bulk materials, the investigation of interfaces often relies on manual, time-consuming methods based on trial and error. I will describe our efforts to implement autonomous workflows for interfaces and integrate them with the design of bulk structures, using our work on understanding and controlling the solid/electrolyte interface in Li-ion batteries as an example. To fully realize the potential of a MAP, a seamless data infrastructure is required, which is capable of handling curated data and metadata from multiple sources and with varying levels of fidelity. At the end of my lecture, I will present our approach to developing such a data infrastructure. This includes achieving complete interoperability of computational workflows and electronic laboratory notebooks from different sources. These involve various simulation engines, time and length scales, and automated data collection and metadata annotation in an ontology-compliant format.