**Automating the virtual discovery of molecules for energy storage**

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**Abstract:**

The further development of existing chemical compounds or the discovery of completely new ones are frequently required for achieving breakthrough advancements. Therefore, the research on the intriguing chemistries of compounds is central to the innovation cycle of new technologies, such as the research on clean energy storage systems. Redox flow batteries are a type of rechargeable batteries where chemical energy is provided by two chemical components, called electrolytes, which are dissolved in liquids that are pumped through the system on separate sides of a membrane. A central issue for developing all-organic redox flow batteries for intermittent renewable electricity storage is the discovery of electrolytes that would satisfy multiple criteria of synthesizability, suitable redox potentials, rapid kinetics, solubility, stability, and safety. An overarching challenge is the speedy identification of useful compounds in an almost infinite chemical space. In this regard, high-throughput computational screening, which relies on robust quantum chemistry methods while utilizing agile software tools on powerful computers, is an insuperable method. In parallel, machine learning methods excel in making fast predictions of material properties and finding insights when they learn from high-quality and large-quantity experimental and computational data. In this course, I will present how computational chemistry and machine learning can be effectively used for the discovery of new electrolytes for energy storage in redox flow batteries. Additionally, I will discuss our efforts on using a combination of physics-based computation, machine learning, and automated vendor search on a systematically generated library of molecules, as well as on the full cell electrochemical characterizations of purchasable and safe compounds from the virtual library. This work therefore is an exemplary application of the high-throughput computational screening guided experiments on a focused chemical space of candidate energy storage materials.