Beyond Crystallinity and Throughput: Machine Learning Accelerated Materials Discovery for Energy Conversion and Storage

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More performant and durable materials are urgently needed to further drive the transition to a sustainable energy system. Unfortunately, accelerated materials discovery is in this field presently still more claim than practical reality. Computational screening approaches hinge on efficient descriptors that only reflect nominal materials properties of the crystalline bulk, simple bulk-truncated surfaces or idealized lattice-matching interfaces. They can thus not account for the substantial, complex and continuous structural, compositional and morphological transitions at the working surfaces or interfaces of catalysts, electrolyzers or batteries. Accelerated experimental discovery in turn still suffers from severe throughput limitations, as easily automatable human steps are rarely limiting the overall workflows. In my talk I will illustrate how modern machine learning (ML) approaches help to overcome these challenges. ML surrogate models, in particular in conjunction with agile active learning-based training, boost the capabilities of predictive-quality multiscale modeling. Starting to tackle the true complexity of working interfaces, the derived mechanistic understanding promises to establish improved descriptors for more reliable computational screening campaigns. For experimental discovery, ML-guided experiment planning allows to optimally use available throughput capacities. In particular most data-efficient adaptive design of experiment (DoE) requires only a limited number of experiments to provide a global (trend) understanding of the materials search space, while simultaneously allowing to batchwise modify and refine both this search space or even the original research objective on the basis of the hitherto accumulated information