When the Algorithms Take Over: AI for Experiment Planning and Control

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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 functional materials in 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 the convergence of AI-based experiment planning and control with automation and robotization is currently starting to change this picture. Examples will not only cover straightforward loop-style self-driving labs for direct exploration of design spaces, but also approaches geared toward mechanistic understanding like automated reaction mechanism generation or autonomous electron microscopy. Methodological frontiers concern significant or varying noise levels (e.g. in case of multi-fidelity measurements), the design of larger numbers of data points (to meet batch-type operation in increasingly parallelized workflows), or agility to either autonomously adapt the shape and dimensions of the search spaces across loops or react to corresponding changes imposed by human scientists.