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Accelerating Perovskite Materials Discovery via High-Throughput Automated Exploration

The intriguing functionalities of metal halide perovskites (MHPs) have led to an extensive exploration of this material for sustainable and scalable optoelectronic applications. However, the inherent chemical complexities in the materials system result in uncontrolled chemical heterogeneities in the synthesized device-grade-level crystalline matrices, which still compromises functionality, and consequently, the performances of the optoelectronic devices. Yet, this phenomenon remains poorly understood due to the massive chemical and synthesis spaces in the complex materials system. In this presentation, an innovative strategy based on a high-throughput automated experimental workflow will be introduced, which is designed to expedite the discovery of fundamental principles and optimized processing pathways in chemically complex perovskite material spaces. Through systematic integration of machine-learning algorithms and/or automated data analysis functionalities, such workflow serves as a powerful tool for constructing the detailed chemical maps of perovskite synthesis, empowering bespoke customization of their structures, dimensionalities, and functionalities. Further, a new concept of co-navigation of theory and experiment spaces accelerating the design of functional perovskites will be proposed. Finally, an outlook of the powerfulness of such automated experimental workflows in accelerating materials discoveries will be illustrated.

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