Improving Lead Halide Perovskite Stability Using Doping and Alloying

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Lead halide perovskites are the main contenders to become next-generation photovoltaics with high efficiency. The major focus is now on improving perovskite stability: organic cations are too volatile, while inorganic Cs is too small to meet the cage size tolerance, and as a result, perovskite converts into a more stable yellow phase. Finding a way to either stabilize the Pb perovskite or completely eliminate the Pb is a high-reward but very challenging problem.

I will discuss our efforts in exploring computationally dopant combinations that could stabilize current state-of-the-art Pb perovskite and then employing high-throughput synthesis procedures to improve the precursors\' solubility and dopability of the perovskite.

An important task is to learn from perovskites and develop new lead-free perovskite-inspired materials with suitable bandgaps for tandem photovoltaics. Existing databases contain several hundred materials with appropriate bandgap, but selecting ones that are easily synthesizable and containing little electronic defects require improvements to existing machine learning models.