

Dream Chemistry Lecture series:

How Physical Chemistry advances Materials Science: solid-state NMR of lead halide perovskites for optoelectronics

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Abstract:

Organic-inorganic lead halide perovskites are a promising family of light absorbers for a new generation of LEDs and solar cells, with reported efficiencies currently exceeding 22%. The field of perovskite photovoltaics is largely driven by systematic optimization of numerous parameters affecting the performance of perovskite solar cells. Such a trial-and-error approach, not backed up by atomic-level understanding of the reasons behind successes and failures, makes rational design of new compositions with better properties extremely difficult.

Here, I will show how we use high-field multi-nuclear (^1H , ^2H , ^{13}C , ^{14}N , ^{15}N , ^{133}Cs , ^{87}Rb , ^{39}K) solid-state magic angle spinning NMR to provide for the first time atomic-level understanding of the different doping strategies used to improve photovoltaic performance of lead halide perovskites. These advances were largely enabled by a new solid-state method of synthesizing highly pure and crystalline lead halide perovskites: *mechanosynthesis*.