

How useful is Solid-State NMR to gain new insights into the structure-property relationship in hybrid perovskites?

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Perovskite solar cells represent one of the most promising photovoltaic technologies, with certified power conversion efficiencies now reaching 27.0%. To fully realize the potential of halide perovskites, it is critical to probe and understand their atomic-level microstructures and structural dynamics, which govern their macroscopic optoelectronic performance and long-term stability.

Solid-state nuclear magnetic resonance (SSNMR) spectroscopy, as a powerful characterization technique, offers unique capabilities to resolve local environments, dynamic processes, and weak interactions within perovskite lattices. Importantly, it allows for the direct quantification of cation reorientational dynamics and lattice fluctuations, which are now increasingly recognized as key factors influencing charge carrier lifetime, trap state density, and phase stability.

By correlating NMR observables with macroscopic device performance metrics, we aim to establish a comprehensive structure–dynamics–property relationship that bridges atomic-scale processes with photovoltaic functionality. This approach will provide new insights for rational perovskite material design and offers atomic-level understanding to guide the further optimization of device performance.

In this presentation, we will highlight recent advances in the NMR field and discuss first results on the NMR signatures of light-induced degradation of $\text{MAPb}(\text{Br}_x\text{Cl}_y\text{I}_z)_3$ when altering the composition with respect to Br, Cl and I. We find clear evidence that the incorporation of iodine leads to destabilization of the halide network upon light exposure.