

Magic Angle Spinning ^{207}Pb and low temperature deuterium NMR as a tool for studying local order and dynamics in $\text{CH}_3\text{NH}_3\text{PbX}_3$ (X=Cl, Br, I) hybrid perovskites

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Presenting high solar energy conversion efficiencies^{1,2} (>21%), hybrid perovskites APbX_3 (A is a small organic cation, X=Cl, Br, I) have recently become one of the most promising material in the field of photovoltaic devices. Meanwhile, fundamental understanding of what makes these preovskites so smart for photovoltaics remains limited. More than three decades ago, Wasylishen *et al.*³ had already revealed the interest of deuterium NMR to investigate the temperature behaviour and the dynamics operating in such materials in their isotropic phase. In fact, solid-state Nuclear Magnetic Resonance (NMR) spectroscopy gives access to the local order and is also a powerful tool to probe dynamical disorder.

Here, we will discuss ^{207}Pb NMR experiments at room temperature on a series of methylammonium lead halides, namely MAPbX_3 with X= Cl, Br and I. The isotropic ^{207}Pb NMR shift is strongly dependent on the nature of the halogen ions and provides a very promising tool for the characterisation of local order in mixed hybrid perovskites. We also confirm the main features of proton, ^{13}C and ^{14}N NMR reported in the litterature^{3,4}. We report on low temperature deuterium NMR, down to 25K, to investigate the structural phase transitions of MAPbBr_3 . The spectra lineshapes below 120K indicates a local disorder of the three-fold axis of the MA cations. It is consistent with the formation of an orientational glass phase, by freezing the dynamical disorder of the high temperature plastic phases.

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