

# What can we learn about lead halide perovskites from infrared spectroscopy?

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Hybrid organic-inorganic perovskites, with the general chemical formula  $ABX_3$  ( $A$  being the organic cation,  $B=Pb$  or  $Sn$ , and  $X$  the halide), exhibit a rich structural and electronic behavior which is strongly influenced by the complex interactions between the organic and inorganic subunits.<sup>1</sup> Hybrid halide perovskites<sup>2</sup> ( $X=Cl, Br, I$ ) were studied in-depth already in the 1990s for their promising opto-electronic properties. Over the last few years the material science community has renewed its interest in the iodide<sup>3-5</sup> and bromide<sup>6</sup> varieties of the methylammonium ( $A=CH_3NH_3^+$ , MA) lead halide perovskites due to their exceptional qualities in photovoltaic applications. While the organic cation does not directly participate in the formation of electronic transport levels, it influences the lattice constants and thereby indirectly the band gap. The dynamic interplay between the rapidly rotating MA cation and the inorganic Pb-X cage is currently under scrutiny,<sup>7,8</sup>

The opto-electronic properties of hybrid perovskites appear to depend strongly on unrecognized details of the fabrication process, leading to a plethora of opposing views in the current literature on several important aspects such as ionic migration. Due to a low formation energy and hence an ease of material decomposition, hybrid perovskites are very susceptible to induced material damages. Infrared (IR) spectroscopy as low energy experimental technique is therefore especially well suited for the physical and chemical characterization of these soft materials.

We will present here how information on the interaction between the organic and inorganic subunits in hybrid perovskites can be inferred from a detailed analysis of IR spectra.<sup>8,9</sup>

Furthermore, we will demonstrate how the impact of external stimuli can be tracked with IR spectroscopy and correlated to electronic properties. We recently found that water can infiltrate methylammonium lead iodide with surprising ease.<sup>10</sup> This infiltration has a strong impact on the opto-electronic properties of the material, possibly via photochemical processes, as demonstrated by measuring the change of photocurrent in lateral devices. Last, we will present an IR spectroscopic study of the influence of above bandgap illumination and surrounding environment on ionic migration in MAPbI.

## References

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