Conference

Structural characterization of halide perovskites by X-ray measurements and advanced analysis.

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The advent of new-generation X-ray sources as well as more sensitive and fast detectors discloses the possibility of deeper static and dynamic structural investigations. X-ray powder diffraction (XPD) and pair distribution function (PDF) measurements are sensitive to long and short-range order, which can be modelled by fitting procedures. Subtle structural changes induced in situ by varying external parameters (temperature, light) can be also detected by processing efficiently multiple measurements. In this case, the traditional approach to fit each measurement independently can be coupled with the new approach to apply multivariate methods to the whole dataset.[1] Single and multiple XPD and PDF measurements have been here analyzed for the high-sensitivity structural characterization of halide perovskites. We have investigated the role played by cyclodextrins (CD) to generate a hybrid perovskite-soft material, demonstrating that the interaction between CDs and perovskite precursors leads to the formation of a supramolecular organic–inorganic hybrid framework that modifies solution chemistry and properties of the perovskite film.**(author?)**[2] The multivariate analysis approach has been applied to *in situ* experiments to reveal under illumination the reversible generation of paramagnetic Pb^{3+} defects in $CH_3NH_3PbI_3$ perovskite (Figure 1),[3] and to get new insights into its tetragonal-to-cubic phase transition under temperature changes.[4]

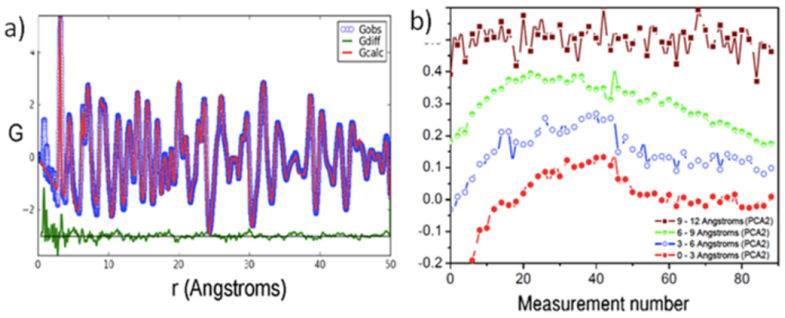

Fig. 1 Fit of the PDF profile (a) and scores obtained by PCA applied to the PDF data matrix in slices of 3Å, for increasing interatomic distances (b).

Riferimenti

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