Experimental report

16/09/2018

Proposal: TEST-2912 **Council:** 4/2018

Title: Excitations in MAPI

Research area:

This proposal is a new proposal

Main proposer: Afonso DA CUNHA FERREIRA

Experimental team: Afonso DA CUNHA FERREIRA

Local contacts: Jacques OLLIVIER

Samples: CH3NH3PbI3

Instrument	Requested days	Allocated days	From	To
IN5	4	4	20/06/2018	24/06/2018

Abstract:

Subject: Structural and dynamic properties of hybrid perovskites for photovoltaic applications.

Proposal: EASY proposal 79417

Team: Afonso Da Cunha Ferreira (LLB and INSA Rennes), Philippe Bourges (LLB), Antoine LéToublon (INSA Rennes), Jacky even (INSA Rennes).

Recently, the three-dimensional hybrid perovskites have conducted to a scientific breakthrough in the quest for low-cost solar cells, with record efficiencies up to 20% [1, 2],. Currently, the state of the art of hybrid organolead perovskites (HOP) solar cells is based on alloys where methylammonium (MA) and formamidinium (FA) are both present in the same structure and ca.10% are replaced by rubidium (Rb) and caesium (Cs) atoms, together with concomitant alloying of iodide (I)/bromide (Br) halogens [3]. The main goal of the PhD project of Afonso Ferreira from LLB-Saclay and FOTON-Rennes, is to better understand the dynamic and structural properties of hybrid perovskites (i.e. low-frequency phonons and relaxation molecular dynamics). In that frame, we have started to look into optical phonons with the purpose of better understanding how the optical and acoustic branches are mixed and how does it affect processes such as up-conversion of low-energy phonons in HOPs.

In the previous EASY access Time of Flight (TOF) experiment at IN5 (TEST-2912), we have looked at the collective dynamics of MAPbI3 over a medium energy range (0-15 meV). The obtained dynamic structure factor S(q,E) is shown in Fig. 1. Overall, the optical phonon spectra in MAPbI3 shows zero to little dispersion. diWe can observe three modes located at around 2.3, 3.8 and 11.7 meV that we have also seen in another inelastic neutron scattering experiment at IN12 (Fig. 2). Recent lattice dynamics calculations indicate that at 2.3 meV correspond to acoustic phonons at the zone boundary, decorated by optical phonons, while the big feature at 11.7 meV should be attributed to incoherent scattering of hydrogen in molecular vibrations [4]. Further analysis of the results are underway.

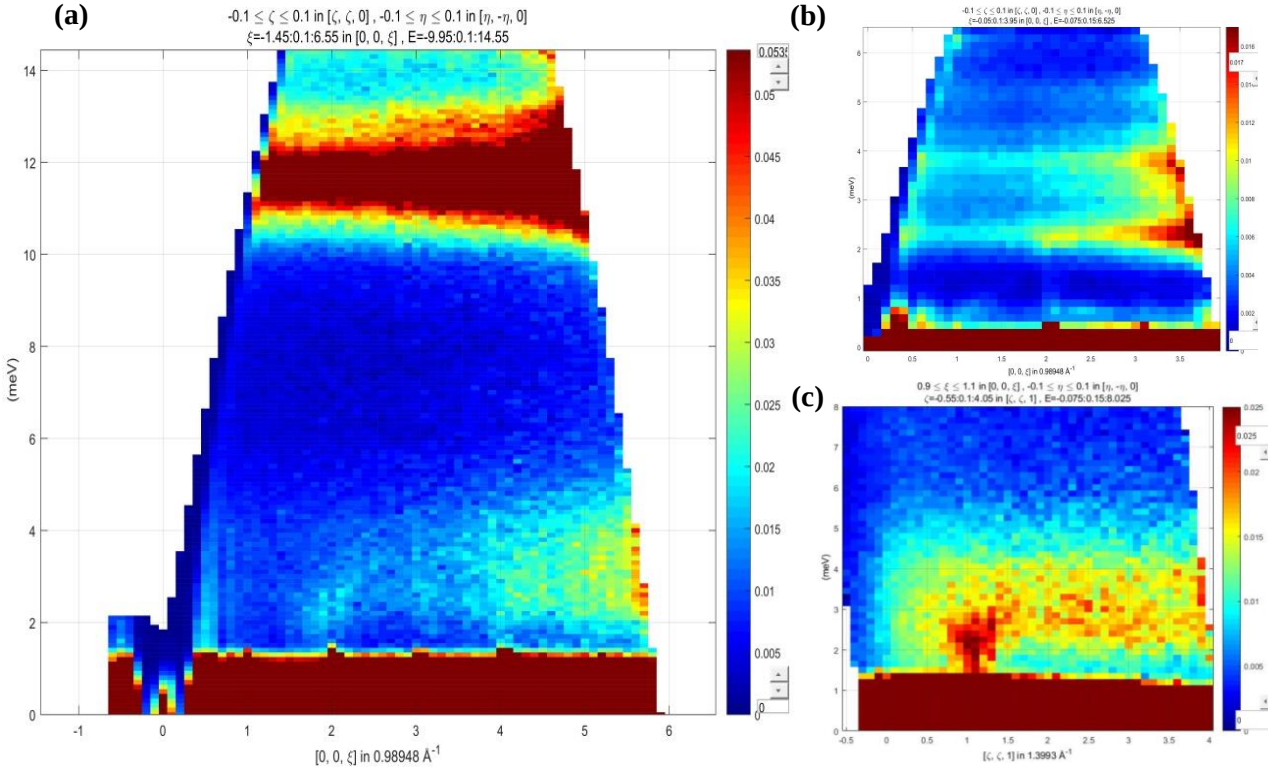

Figure 1. *S(q,E) contour plot of the phonon spectra at 5 K, obtained with λ = 2 Å,* ***(a)*** *along [00l] and (c) along [hh0] around the (111) bragg reflection.* ***(b)*** *Contour plot of the phonon spectra at 5 K, obtained with λ = 3 Å, zoomed it on the low energy modes of Figure 1a.*

References

1. A. Kojima *et al.*, J. Am. Chem. Soc. 131, 6050 (2009).
2. NREL chart, https://www.nrel.gov/pv/assets/pdfs/pv-efficiencies-07-17-2018.pdf
3. M. Saliba *et al.*, Science 354(6309), 206 (2016).
4. Bing Li *et al.*, Nat. Comm. 8, 16086 (2017).