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Phonons in hydrid perosvkites

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Hybrid organolead perovskites (HOP) have started to establish themselves in the field of photovoltaics, mainly due to their great optoelectronic properties and steadily improving solar cell efficiency. Although much recent attention has been devoted towards unraveling their microscopic optoelectronic properties, the structural dynamics (phonons) are currently still lacking a comprehensive understanding as compared to that already reached for classic semiconductors. Study of the lattice dynamics is then a key in understanding the electron-phonon interactions at play, responsible for the electronic properties. Using inelastic neutron scattering and light (Brillouin and Raman) scattering, we have investigated the phonon spectrum in four different hybrid perovskite single crystals: MAPbBr3, FAPbBr3, MAPbI3 and α-FAPbI3, where MA and FA correspond to methylammonium (CH3NH3) and formamidinium ((CH2)2NH) molecules, respectively.
Previously, we have studied the low energy acoustic phonons and determine the complete set of elastic constants [1,2]. They are characterized by soft elastic constants compared to classic semiconductors, with a particular very soft shear modulus C44. Between room temperature and 240 K, a tendency towards an incipient ferroelastic transition is also observed in FAPbBr3. A systematic lower sound group velocity is found in the technologically important iodide-based compounds compared to the bromide-based ones. The findings suggest that low thermal conductivity and hot phonon bottleneck phenomena are expected to be enhanced by low elastic stiffness, particularly in the case of the ultrasoft α-FAPbI3
Recently, we investigated the optical phonon spectrum below 40 meV in single crystals of the same four different hybrid lead halide perovskites [3]. Low temperature spectra reveal weakly dispersive optical phonons, grouped in three main bundles of phonons (see figure). These results will be discussed showing that the lowest energies phonons at 2-5 meV seem to be the origin of the limit of the charge carrier mobilities in these materials. The temperature dependence of the neutron spectra reveals a significant anharmonic behaviour, resulting in optical phonon overdamping at temperatures as low as 80 K, questionning the validity of the quasi-particle picture for the low energy optical modes at room temperature where the solar cells actually operate.

[1] A. Létoublon et al., Journal of Phys. Chem. Lett. 7, 3776 (2016).
[2] A.C. Ferreira et al, Phys. Rev. Lett 121, 085502 (2018).
[3] A.C. Ferreira et al, Communications phys. 3,48 (2020) https://arxiv.org/abs/2001.05445

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