Title: Elastic softness of hybrid lead halide perovskites

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Content:

Hybrid organic-inorganic perovskites have been intensively studied as promising materials for photovoltaic applications, taking advantage of their high efficiency and low cost processing. Although much recent attention has also been devoted towards unraveling their microscopic optoelectronic properties, the origin of their softness, by comparison to classic semiconductors, is currently still lacking a comprehensive understanding and systematic experimental studies. Here we investigate by coherent inelastic neutron scattering spectroscopy and Brillouin light scattering, low frequency acoustic phonons in four different hybrid perovskite single crystals: MAPbBr₃, FAPbBr₃, MAPbI₃ and α -FAPbI₃. We report a very small shear C₄₄ elastic constant for all the compounds and a considerable elastic anisotropy. The extremely low bulk modulus and negative C₁₂ in α -FAPbI₃ substantiates its very unstable nature and in FAPbBr₃, a tendency towards an incipient ferroelastic transition, is interpreted as further evidence of the influence of plasticity in hybrid perovskites. We observe a systematic lower sound group velocity 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.

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