Title: Stress effects on vibrational spectra of orthorhombic and tetragonal hybrid perovskites.

Authors: Kuntal Talit and David A. Strubbe
Affiliation: Department of Physics, University of California, Merced

Strain plays an important role in semiconductor performance and stability. Strains may develop in organic metal-halide perovskites which affect carrier mobility, non-radiative recombination, degradation and other optoelectronic properties. Measuring spatially varying strains is difficult but imperative for understanding these effects. Previously we have looked into high temperature pseudo-cubic phase [arXiV:1907.03673]. In this work, we have used DFT to investigate effects of applied strain on the vibrations of tetragonal and orthorhombic methylammonium lead iodides (MAPI) via Raman spectroscopy. Applying small uniaxial strains along three crystal axes we have analyzed changes in frequency and phonon displacement patterns. By analyzing the changes in dynamical matrices, we are able to understand different atomic interactions that are significant for the mode frequency change under strain. We identified favorable modes for experimental measurements. Our study gives insight into the interaction between strain, structural changes and vibrational modes which may help to understand degradation.

Funding acknowledgement: computing time on MERCED cluster at UC Merced and NERSC supercomputer at LBNL.