

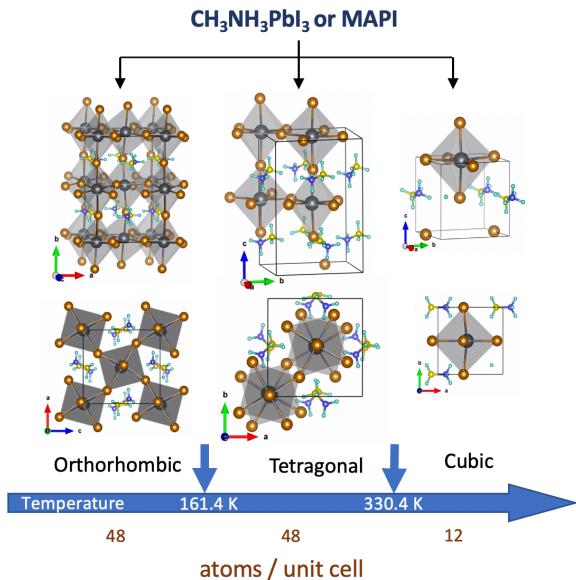
Stress effects on vibrational spectra of hybrid perovskite: A probe of local strain



Kuntal Talit and David A. Strubbe

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Methylammonium Lead Iodide

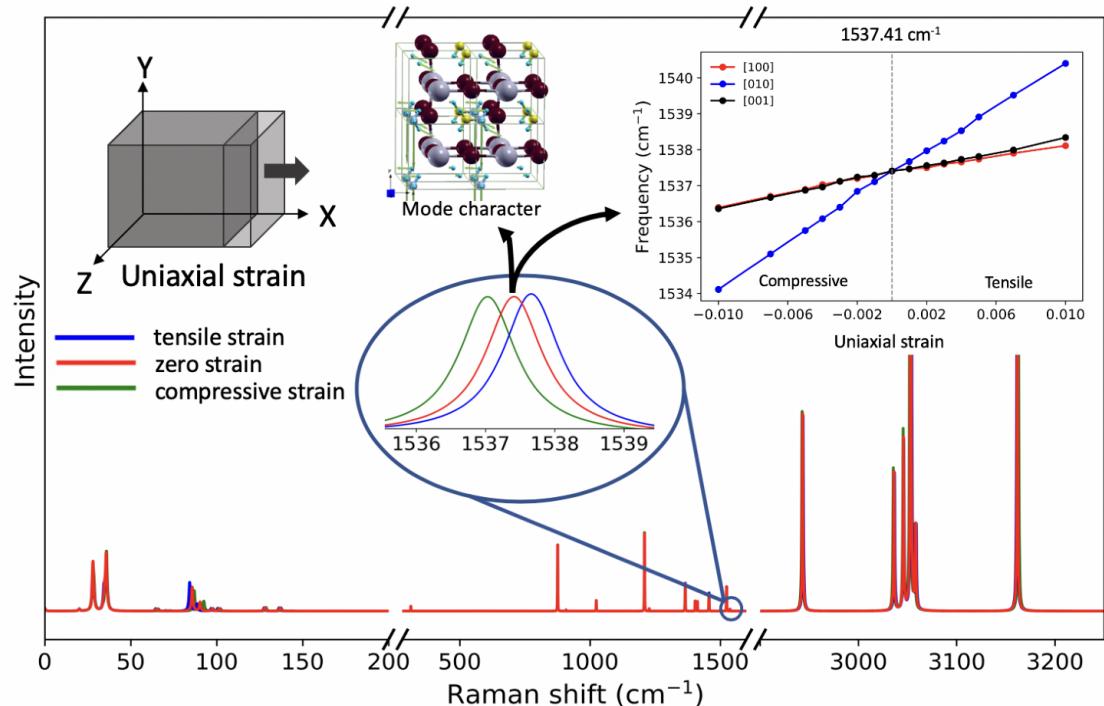


Quantum-Espresso code is used to do all DFT and DFPT calculations.

<http://www.quantum-espresso.org>

P. Giannozzi et al., J. Phys. Condens. Matter **21** 395502 (2009)

How Raman spectra can be used to measure localized strain in perovskites



K. Talit et al., arXiv:1907.03673

- Does all the modes behave similarly under strain?
- What are the reasons behind different shift patterns?
- What are the best possible Raman and IR modes for doing experiment?
- How structural changes and changes in dynamical matrices can help us to understand the effect of strain on vibrational spectra?

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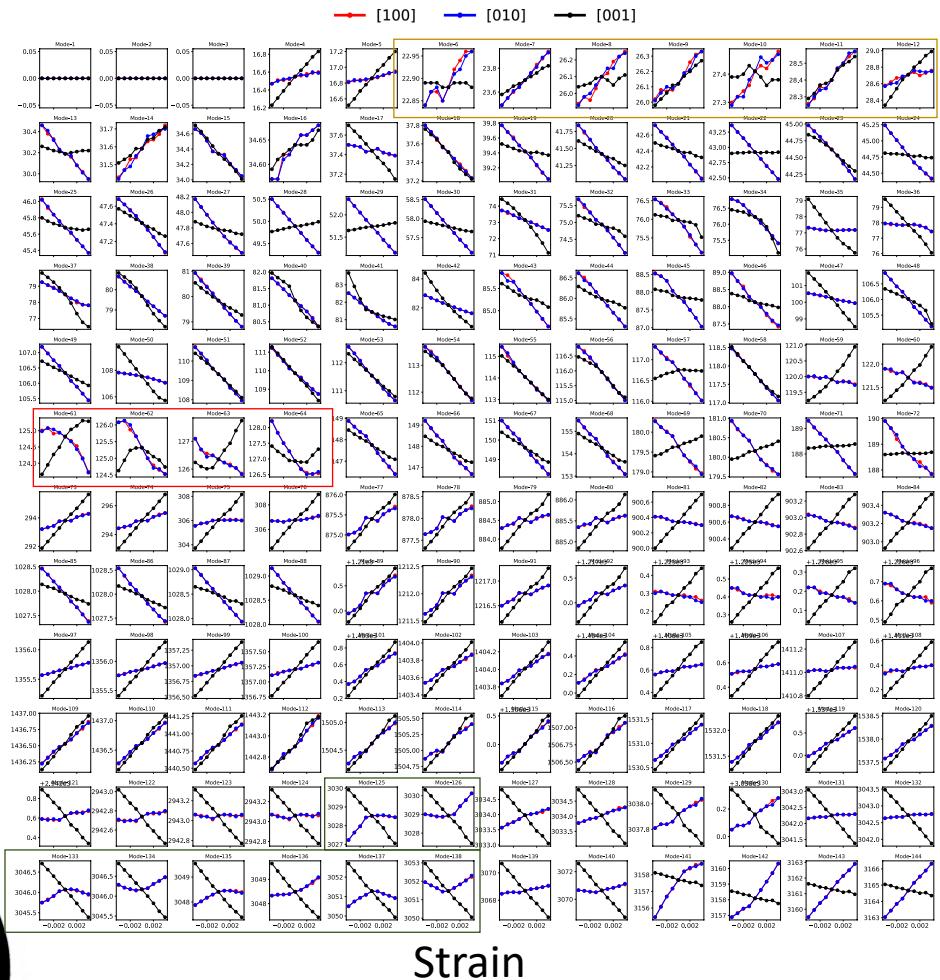
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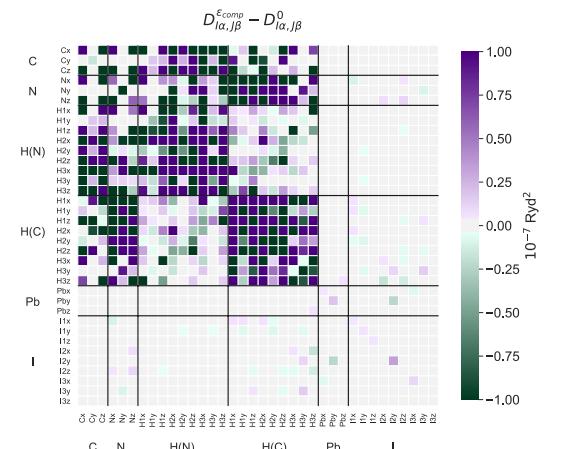
Type of challenges:

Change in frequency with strain for tetragonal MAPI

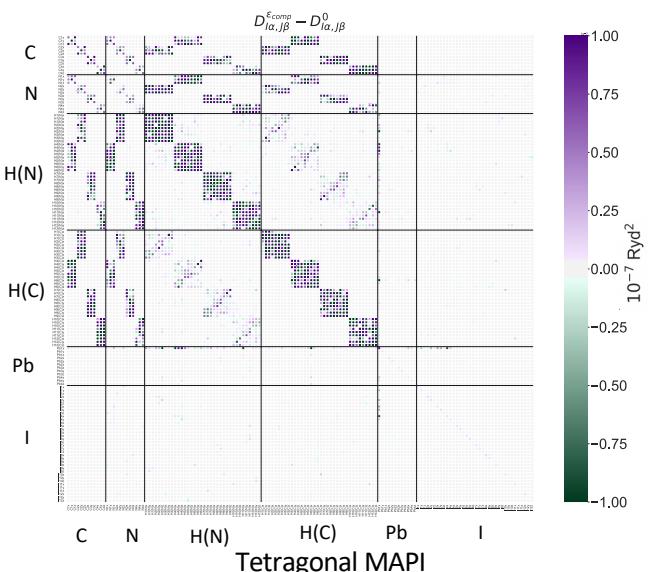
Frequency in cm^{-1}



Change in dynamical matrix



Cubic MAPI



MERCED Cluster

NERSC