

Supplementary Material

Raman Spectroscopy of Lithium Niobite (LiNbO₂)

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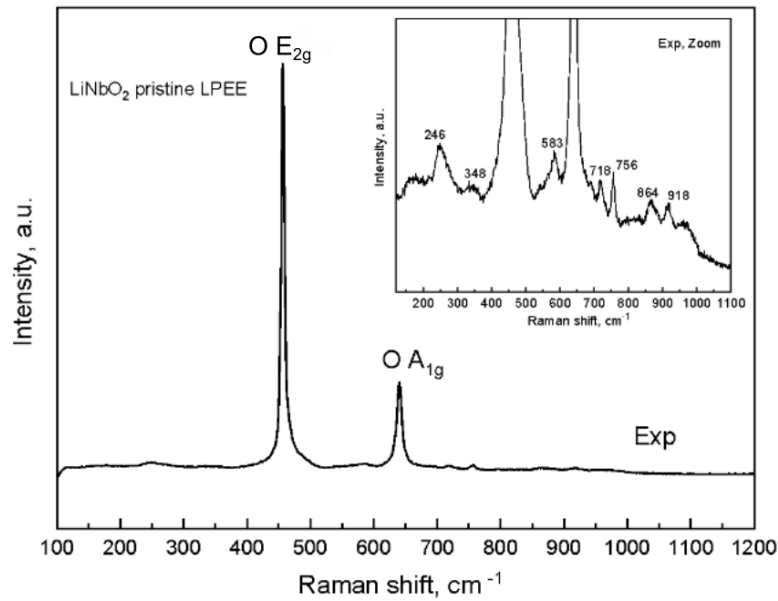


FIG. S1 Raman spectra of pristine LiNbO₂. Inset shows zoomed in spectra exhibiting less pronounced peaks.

Mode symmetry, D_{6h}(6/mmm) point group:

freq (1 - 2) =	-2.9 [cm-1]	--> E _{1u}	I
freq (3 - 3) =	4.2 [cm-1]	--> A _{2u}	I
freq (4 - 5) =	53.5 [cm-1]	--> E _{2g}	R
freq (6 - 6) =	128.6 [cm-1]	--> B _{1g}	
freq (7 - 8) =	150.5 [cm-1]	--> E _{2u}	
freq (9 - 10) =	155.1 [cm-1]	--> E _{1u}	I
freq (11 - 11) =	347.6 [cm-1]	--> A _{2u}	I
freq (12 - 13) =	417.5 [cm-1]	--> E _{2u}	
freq (14 - 15) =	422.5 [cm-1]	--> E _{1g}	R
freq (16 - 17) =	455.1 [cm-1]	--> E _{1u}	I
freq (18 - 19) =	458.2 [cm-1]	--> E _{2g}	R
freq (20 - 20) =	483.0 [cm-1]	--> B _{2u}	
freq (21 - 21) =	630.3 [cm-1]	--> A _{2u}	I
freq (22 - 22) =	638.1 [cm-1]	--> A _{1g}	R
freq (23 - 23) =	666.1 [cm-1]	--> B _{2u}	
freq (24 - 24) =	699.7 [cm-1]	--> B _{1g}	

FIG. S2 List of infrared active and raman active modes for LiNbO_2

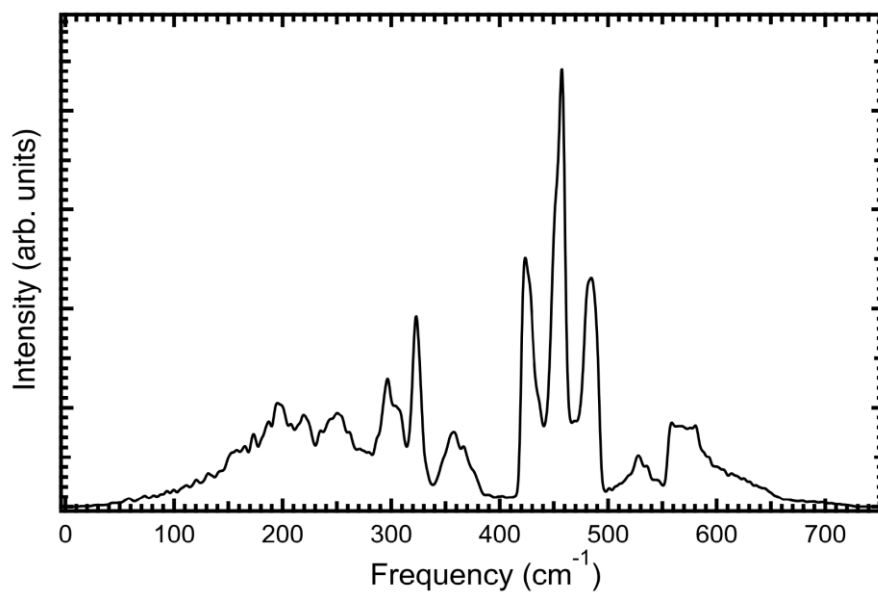


FIG. S3 Total phonon density of states of stoichiometric LiNbO_2 .

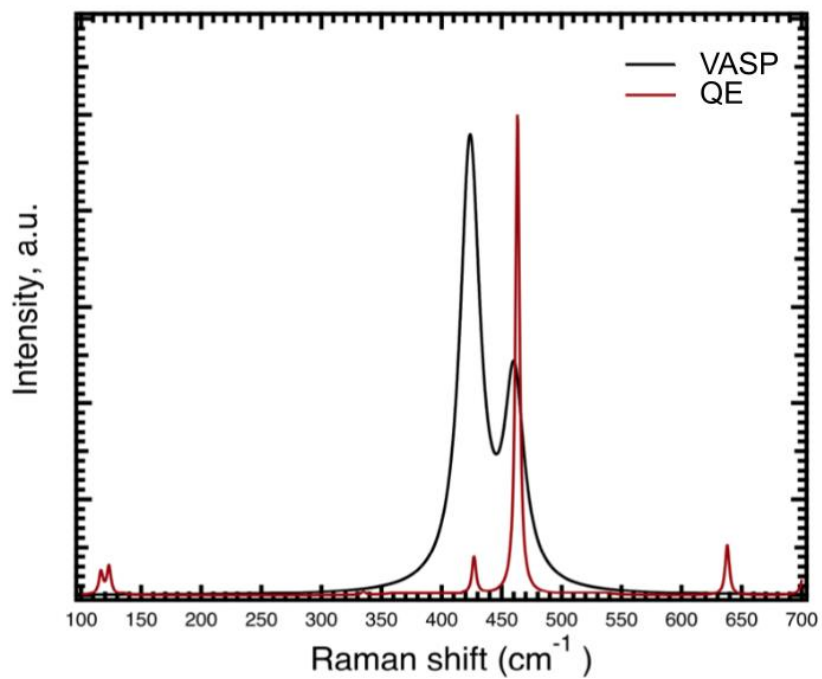


Fig.S4. Simulated Raman spectra using QE and VASP.

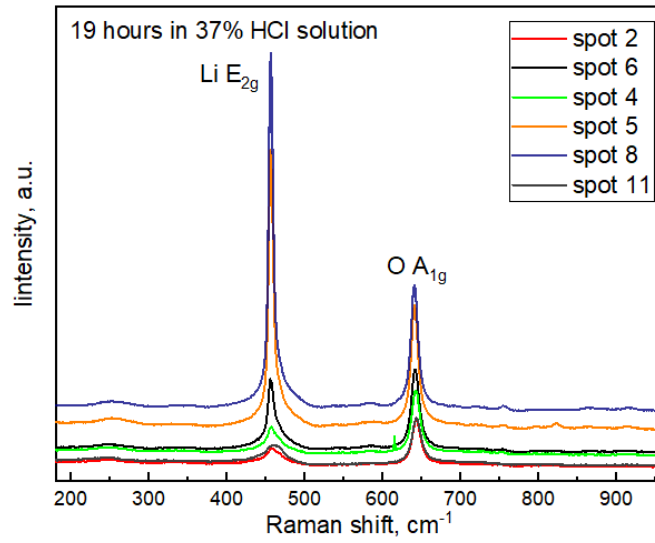


FIG. S5 Spot sensitivity of Raman spectra for HCl soaked LiNbO₂.