Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Ab initio DFT calculations of vibrational properties[1] S.M. STORY, F.D. VILA, J.J. KAS, J.J. REHR, Univ of Washington — Vibrational properties such as EXAFS and crystallographic Debye-Waller factors, vibrational free energies, phonon self-energies, and phonon contributions to the electron spectral function, are key to understanding many aspects of materials beyond ground state electronic structure. Thus, their simulation using first principles methods is of particular importance. Many of these vibrational properties can be calculated from the dynamical matrix and electron-phonon coupling coefficients obtained from DFT calculations. Here we present a code DMVP [1] that calculates these properties from the output of electronic structure codes such as ABINIT, Gaussian, Quantum Espresso and VASP. Our modular interfacing tool AI2PS allows us to translate the different outputs into a DMVP compatible format and generate vibrational properties in an automated way [2]. Finally, we present some current applications that take advantage of the modular form of AI2PS to extend its capabilities to the calculation of coefficients of thermal expansion and other properties of interest such as infrared spectra.

[1] F. D. Vila et al., Phys. Rev. B **76**, 014301 (2007).
[2] J.J. Rehr et al., C. R. Physique **10** (2009).

[1]This work was supported by DOE Grant DE-FG02-97ER45623.

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Date submitted: 15 Nov 2013 Electronic form version 1.4