Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Calculation of Raman and infrared spectra by coherent-phonon stimulation JONATHAN YATES, IVO SOUZA, University of California, Berkeley and Lawrence Berkeley National Laboratory — We propose a novel method for the efficient first principles prediction of Infra-Red and non-resonant Raman spectra. The method is inspired by the experimental technique of impulsive- stimulated Raman scattering. We apply initial impulsive forces to the ions in the system. For IR spectroscopy these forces correspond to the first order forces induced by a static electric field; for Raman spectroscopy they are the second order forces. We show how the corresponding vibrational spectrum can be obtained from the ensuing short-time dynamics of the system. The method has better scaling with system size than existing techniques. We present applications of the method to various clusters and molecules.

Jonathan Yates
University of California, Berkeley and Lawrence Berkeley National Laboratory

Date submitted: 03 Dec 2004 Electronic form version 1.4