Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization[1] MARIOS ZACHARIAS, FELICIANO GIUSTINO, University of Oxford — Electron-phonon interactions are of fundamental importance in the study of the optical properties of solids at finite temperatures. Here we present a new first-principles computational technique based on the Williams-Lax theory for performing predictive calculations of the optical spectra, including quantum zero-point renormalization and indirect absorption [1]. The calculation of the Williams-Lax optical spectra is computationally challenging, as it involves the sampling over all possible nuclear quantum states. We develop an efficient computational strategy for performing "one-shot" finite-temperature calculations [2]. These require only a single optimal configuration of the atomic positions. We demonstrate our methodology for the case of Si, C, and GaAs, yielding absorption coefficients in good agreement with experiment. This work opens the way for systematic calculations of optical spectra at finite temperature. [1] M. Zacharias, C. E. Patrick, and F. Giustino, Phys. Rev. Lett. 115, 177401 (2015). [2] M. Zacharias and F. Giustino, Phys. Rev. B 94, 075125 (2016).

[1]This work was supported by the UK EPSRC (EP/J009857/1 and EP/M020517/) and the Leverhulme Trust (RL-2012-001), and the Graphene Flagship (EU-FP7-604391).

MARIOS ZACHARIAS
University of Oxford

Date submitted: 04 Nov 2016 Electronic form version 1.4