Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electron-phonon coupling using many-body GW theory[1] BARTOMEU MONSERRAT, DAVID VANDERBILT, Rutgers University — Electron-phonon coupling drives a plethora of phenomena, such as superconductivity in metals, or the temperature dependence of optical properties in semiconductors. There is increasing evidence that semi-local density functional theory (DFT) is not adequate for the description of electron-phonon coupling, and instead effects such as electronic correlation need to be included. Unfortunately, methods beyond semi-local DFT are computationally demanding, limiting the study of these phenomena. In this talk we will introduce the idea of "thermal lines", which can be used to explore the vibrational phase space of solids and molecules at small computational cost. In particular, we will describe how thermal lines can be exploited to calculate the temperature dependence of band structures beyond semi-local DFT, by using many-body GW theory, or by including the effects of spin-orbit coupling. We will present first-principles results showing the effects of electron correlation on the strength of electron-phonon coupling, and the effects of electron-phonon coupling on topological states of matter.

[1]Supported by Robinson College, Cambridge, and the Cambridge Philosophical Society.

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Date submitted: 03 Nov 2015 Electronic form version 1.4