Abstract Submitted for the MAR15 Meeting of The American Physical Society

Is Sodium a Superconductor Under Pressure? ROXANNE TUTCH-TON, The Colorado School of Mines, XIAO-JIA CHEN, The Carnegie Institution of Washington, ZHIGANG WU, The Colorado School of Mines — Superconductivity has been discovered in compressed Li with a critical temperature ( $T_c$ ) of 14 K. The other alkali metals are, theoretically, predicted to become superconductors under pressure. Sodium (Na) is the notable exception. Previous *ab initio* calculations considered superconductivity only in the BCC and FCC structures of alkali metals; however, Na goes through complicated, structural phase transitions at higher pressures until it becomes an insulator around 260 GPa. We have performed firstprinciples linear response calculations for four metallic phases (BCC, FCC, cI16 and tI19) of Na to compute lattice dynamics and the electron-phonon spectral function. The electron-phonon coupling parameter as well as  $T_c$  were then determined as functions of pressure to a maximum  $T_c$  of 1.2 K in the cI16 phase, then it decreases rapidly to zero K at higher pressures.

> Roxanne Tutchton The Colorado School of Mines

Date submitted: 12 Nov 2014

Electronic form version 1.4