Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Electron-Phonon Renormalization of Band Gap of BN and Si nanowires ANDREW FRANSON, Colorado Sch of Mines — We compute the electron-phonon renormalization of band gap of BN with three different crystal structures from first-principles using the linear-response theory and the Allen-Heine theory. We find that the zero-point renormalization of band gap in BN depends strongly on crystal structures, varying from -222 meV to -434 meV. We also calculate the temperature-dependent band gaps and electronic band structures of BN. In addition, we investigate the quantum confinement effect on electron-phonon renormalization by comparing band gap shifts due to electron-phonon coupling in bulk Si and Si nanowires.

Andrew Franson
Colorado Sch of Mines

Date submitted: 15 Nov 2013 Electronic form version 1.4