Abstract Submitted for the MAR16 Meeting of The American Physical Society

First-principles calculation of LO phonon scattering in $BaSnO_3^1$ KARTHIK KRISHNASWAMY, BURAK HIMMETOGLU, ANDERSON JAN-OTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — BaSnO₃ (BSO) has drawn interest owing to the recent discovery of high electron mobility, highest among the perovskite materials. In our theoretical work, we calculate the electron scattering rate due to LO phonon scattering from first-principles density functional calculations. The calculated mobility is much higher than the experimentally observed value, suggesting defect scattering as the primary limiting factor in currently grown BSO samples, and that reducing the defect density can enhance BSOs mobility significantly.

¹This work was supported by the LEAST Center and by ONR.

Karthik Krishnaswamy University of California, Santa Barbara

Date submitted: 03 Nov 2015

Electronic form version 1.4