

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First principles and force field calculations of thermal transport in bulk semiconductors and oxides: a comparative study¹ EAMONN MURRAY, UC Davis, IVANA SAVIC, Tyndall National Institute, Cork, Ireland, GIULIA GALLI, UC Davis — At present, large scale calculations of thermal transport properties of materials are carried using empirical potentials², due to difficulties in scaling ab initio methods to directly compute the thermal conductivity of complex, nanostructured systems. It is therefore important to assess the predictive ability of empirical potentials for representative bulk systems, for which ab initio simulations are possible, and to establish their accuracy in yielding absolute values of computed thermal conductivities (κ) and trends within given classes of systems. We report on comparisons between thermal conductivities of elemental semiconductors and insulators (Si, C, Ge) and simple oxides (MgO and SiO₂) as obtained using the Boltzmann Transport equation with first principles, DFT Hamiltonians and Tersoff type empirical potentials. The second and third derivatives of the energy with respect to atomic displacements are obtained by finite difference calculations in supercells in all cases. A detailed discussion of the reasons why these empirical potentials appear to systematically overestimate κ will be presented.

¹Work supported by DOE-BES grant no. DE-FG02-06ER46262.

²See, e.g. Y.He, I.Savic, D.Donadio and G.Galli PCCP 2012 ASAP (DOI: 10.1039/C2CP42394D)

Eamonn Murray
UC Davis

Date submitted: 09 Nov 2012

Electronic form version 1.4