

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Atomistic quantum thermal conductance profile of hybrid interfaces JEEVAKA WEERASINGHE, Department of Physics, University of North Texas, Denton, TX 76203, ARRIGO CALZOLARI, Istituto Nanoscienze CNR-NANO S3 Center, I-41125 Modena, Italy, MARCO BUONGIORNO NARDELLI, Department of Physics and Department of Chemistry, University of North Texas, Denton, TX 76203 — Atomistic structure at interfaces has been shown to play a critical role in quantum thermal conductance across nanoscale interfaces. In general, current models derive phonon transmission probabilities from bulk material properties. However, they do not account for the effect of atomic scale interfacial structure on thermal conductance. Here we use an ab initio approach that we have recently developed to investigate the correlation between interfacial atomic structure and quantum thermal conductance. In particular, we will discuss the electronic structure and thermal conductances in systems with hybrid metal/self-assembled monolayer (SAM) interfaces with varying chemistry in order to elucidate the role of metal-organic bonds in the thermal properties of complex assemblies. Our methodology integrates the accurate self-consistent minimization of the ground state electronic structure via first-principles density functional theory based calculations, the determination of interatomic force constants via density functional perturbation theory, and the calculation of the quantum conductance using a real space Green's function formalism based on the Landauer approach.

Jeevaka Weerasinghe
Department of Physics, University of North Texas, Denton, TX 76203

Date submitted: 09 Nov 2012

Electronic form version 1.4