

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First principles calculations of thermal conductivity with out of equilibrium molecular dynamics simulations¹ MARCELLO PULIGHEDDU, Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis, CA 95616, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637 and Materials Science Division, Argonne National Laboratory, Lemont, IL — The prediction of the thermal properties of solids and liquids is central to numerous problems in condensed matter physics and materials science, including the study of thermal management of opto-electronic and energy conversion devices. We present [1] a method to compute the thermal conductivity of solids by performing ab initio molecular dynamics at non equilibrium conditions. Our formulation is based on a generalization of the approach to equilibrium technique, using sinusoidal temperature gradients, and it only requires calculations of first principles trajectories and atomic forces. We discuss results and computational requirements for a representative, simple oxide, MgO, and compare with experiments and data obtained with classical potentials. [1] M. Puligheddu et al. Submitted 2016

¹This work was supported by MICCoM as part of the Computational Materials Science Program funded by the U.S. Department of Energy (DOE), Office of Science , Basic Energy Sciences (BES), Materials Sciences and Engineering Division under grant DOE/BES 5J-30

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Date submitted: 09 Nov 2016

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