Abstract Submitted for the MAR14 Meeting of The American Physical Society

Thermal transport in nanostructured silicon membranes<sup>1</sup> SANG-HAMITRA NEOGI, LUIZ F.C. PEREIRA, DAVIDE DONADIO, Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — The recent focus in thermal management in nanostructures and energy harvesting using thermolectric devices has motivated the interest towards understanding the role of phononic thermal transport in these nanoscale materials. One way to obtain thermoelectric systems with improved efficiency is to engineer nanostructured semiconductors, so as to reduce the thermal conductivity of the crystalline materials while preserving their electronic properties [1]. Our study is driven towards understanding the nature of phononic thermal transport in nanostructured silicon membranes. We use harmonic lattice dynamics and classical molecular dynamics to compute the phonon transport properties in Si membranes, with thickness up to 20 nm. We show that dimensionality reduction has a significant effect on the vibrational properties and leads to a 4-fold reduction in the thermal conductivity of the membranes. Combining dimensional reduction with surface modification, we obtain a reduction in the thermal conductivity of the membranes to a factor of 20 with respect to the bulk, implying a 20-fold enhancement of ZT at room temperature. Such figures make nanostructured silicon membranes viable materials for thermoelectric units. [1] M. S. Dresselhaus et al, Adv. Mater., 22, 3970 (2010).

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