

Abstract Submitted
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Heat Flow in Heterostructures MEHMET BEBEK, STEFAN ESTRE-
ICHER, Texas Tech University — Existing theoretical descriptions of thermal trans-
port through heterostructures describe the process in terms of empirical reflection
and transmission. First-principles theoretical tools are required to describe at the
atomic level the flow of heat at the boundary between two materials. The interac-
tions between the (localized) phonons associated with the interface and the (delocal-
ized) bulk phonons can be described using ab-initio molecular-dynamics simulations
provided that temperature fluctuations are controlled without using a thermostat.
This can be achieved by preparing the supercell using the eigenvectors of the dy-
namical matrix. Our approach and preliminary results dealing with a Ge layer in a
Si nanowire will be discussed.

Mehmet Bebek
Texas Tech University

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