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Atomistic design of semiconductor nanostructures with optimal thermoelectric properties[1]

GIULIA GALLI, University of California Davis

The search for novel materials with optimal thermoelectric properties (for either thermoelectric power generation or heat dissipation) is an active field of research. We present atomistic and *ab-initio* simulations of selected nanomaterials, aimed at predicting thermal conductivities and electronic transport properties, and ultimately at designing materials with optimal thermoelectric figure of merit. In particular we focus on carbon nanotubes [1], silicon wires [2] and nanoporous silicon [3] and we discuss both strategies and algorithms to optimize thermoelectric properties at the nanoscale.

[1] D. Donadio and G.Galli, Phys. Rev. Lett. 2007 (in press).
[2] T.Vo, A.Williamson, V.Lordi and G.Galli (submitted) and J.Reed, A.Williamson, E.Schwegler and G.Galli (submitted).
[3] J.-H. Lee, J.C.Grossman, J.Reed and G.Galli, Appl. Phys. Lett. 2007 (in press).

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