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First-principles Theory of Inelastic Transport and Local Heating in Atomic Gold Wires

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ABSTRACT

Thomas Frederiksen, Magnus Paulsson, Mads Brandbyge, and Antti-Pekka Jauho
MIC — Department of Micro and Nanotechnology, NanoDTU, Technical University of Denmark, Ørsteds Plads, Bldg. 345E, DK-2800 Lyngby, Denmark

We present theoretical calculations of the inelastic transport properties in atomic gold wires. Our method is based on a combination of density functional theory and non-equilibrium Green's functions. The vibrational spectra for extensive series of wire geometries have been calculated using SIESTA, and the corresponding effects in the conductance are analyzed. In particular, we focus on the heating of the active vibrational modes. By a detailed comparison with experiments we are able to estimate an order of magnitude for the external damping of the active vibrations. ©2007 American Institute of Physics

KEYWORDS and PACS

Keywords

electron transport theory, gold, density functional theory, Green's function methods

PACS

- 72.10.Bg
  General formulation of electronic transport theory
- 72.15.Eb
  Electrical and thermal conduction in crystalline metals and alloys
- 71.15.Mb
  Density functional theory, local density approximation, gradient and other corrections (condensed matter electronic structure)

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