Carl von Ossietzky
Universität
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Institut für PHYSIK

Theoriekolloquium

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https://meeting.uol.de/b/and-etc-jmj-1y9

Am **1. Juli 2021 um 14.15 Uhr** hält

Herr Dr. Samy Merabia (Lyon)

einen Vortrag mit dem Titel

Thermal transport across nanoscale vacuum gaps and across single molecule junctions

Heat can be transferred between two objects by conduction or by radiation. Conduction is the mode of transfer between objects in contact while thermal radiation describes long-range heat transfer in the absence of contact. At nanoscale separation scales (extreme near field), however, the distinction between conduction and radiation becomes somewhat blurred. Very recent experiments perfomred at the university of Oldenburg, have shown that heat transfer between two gold surfaces separated by a few nanometers exceeded near field radiation transfer by several orders of magnitude [1]. These results showed discrepancies with the conventional theory which considers only photon as near field energy carriers. In parallel, the thermal conductance of single molecule junctions has been recently determined experimentally [2,3] opening the door to confirm the high thermoelectric efficiency displayed by these nano-objects. All these experiments call for models capable of describing accurately thermal transport by phonon, phonon or electrons across nanoscale gaps or molecules.
In this contribution, we model heat transfer across nanometer gaps and across single-molecule junctions using a combination of different atomistic simulations (molecular dynamics and ab-initio calculations). First, we demonstrate [4] that phonons dominate heat transport at nanometer distances, even in the presence of molecules in the gap [5]. This conclusion is shown to hold for nanogaps separating different types of materials. The computed thermal conductance levels turn out to be several orders of magnitude higher than the predictions of acoustic continuous models. These discrepancies stem from the contribution of intermediate phonon frequencies which are not accurately described by acoustic models. Moreover, we highlight the leading role played by phonon scattering as compared with electron tunneling and electron/phonon processes at interfaces [6].

The second issue to be discussed concerns thermal transfer across molecular junctions [7]. We consider junctions made of OPE3 derivatives, as these molecules are commonly synthesized by experimentalists and already extensively studied for electronic transport. The phonon thermal conductance of the corresponding gold-molecule-gold junctions are computed here using atomistic calculations. For Au-OPE3-Au junctions, the computed thermal conductance obtained is in good agreement with the experimental value [3]. Next, we characterize the phonon thermal conductance of cross linked molecules junctions, as a function of their length and the nature of the cross-linker. In particular, we show that constrained cross-linked molecules display relatively low thermal conductance, which makes them promising for thermoelectric applications. These low conductance levels are interpreted based on phonon transmission calculations.

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Interessierte sind herzlich eingeladen.

gez. PD Dr. Svend-Age Biehs