THERMAL CONDUCTIVITY FROM QUANTUM MOLECULAR DYNAMICS

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : Institut Lumiere Matiere

LEVEL : M2
TEAM(S) : MMCI

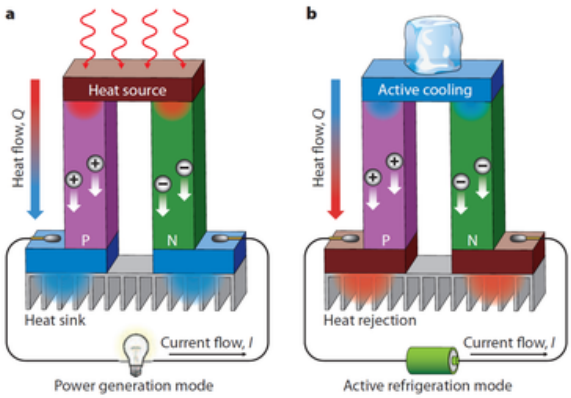
CONTACT(S) : NIEHAUS Thomas

CONTACT(S) DETAILS: thomas.niehaus[at]univ-lyon1.fr / Tel. 0472431571

KEYWORD(S) : Modeling / DFT / Ab-initio

SCIENTIFIC CONTEXT :

The direct conversion of a temperature gradient to electric voltage or vice versa is known as the thermoelectric effect. Although first rigorously defined following a series of discoveries in the mid 19th century, it was not until the mid 20th century that materials exhibiting interesting thermoelectric properties were sufficiently understood to enable targeted research. Today, anthropogenic waste heat contributes significantly to climate change and for economic, as well as environmental reasons, creates a strong imperative to develop new thermoelectric materials. Recently, downsizing of devices up to the molecular limit has shown to be an effective measure to increase performance. The characteristic figure of merit for thermoelectric materials is typically denoted ZT, and depends on the thermal conductivity of the material. The standard way to obtain this quantity is to perform molecular dynamics simulations based on empirical potentials.



From Li et al., NPG Asia Mater 2, 152 (2010)

MISSIONS :

In this project, we attempt to evaluate the thermal conductivity using first principles methods (density functional theory) by performing quantum molecular dynamics. This approach should be more transferable and provide higher transferability, but is limited to small devices. The thesis will compare the two approaches for molecular junctions comprised of an organic molecule bridging two metal electrodes. One further goal is to quantify which vibrational modes of the molecule contribute most to the thermal conductivity.

OUTLOOKS :

This internship can be extended into a PhD.

published on 31/07/2024