Atomistic simulations of nanoscale heat flow

Supervision: Dvira Segal (dvira.segal@utoronto.ca)
https://sites.chem.utoronto.ca/chemistry/dsegal

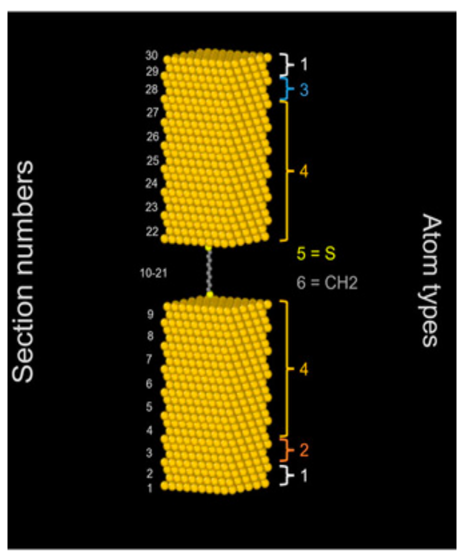
Topic: The goal of this research is to understand mechanisms of thermal energy flow in atomistic/molecular-based nanojunctions, learn how to manipulate heat flow at the nanoscale, propose nanoscale thermal devices with nonlinear function (such as thermal diodes), and guide experimental work [1].

Method: We are using classical molecular dynamics (MD) simulations to study phononic heat transfer across interfaces and single molecules. As described in Ref. [2], we had recently developed protocols for computing phononic heat currents at the nanoscale.

Objectives for summer projects: This project will build on our recent publication [2]. The student will study one (or more!) of the following questions:
(i) When and why does the nanoscale system display an anomalous equilibration dynamics?
(ii) Are there cooperative (nonadditive molecular) effects in nanoscale thermal transport?
(iii) What are the dominant transport mechanisms through systems that are not quasi one-dimensional, rather e.g., involving torsional motion or are spherical, such as fullerenes?
(iv) How do we integrate machine-learning potentials into our simulation protocol?

Tasks: The summer student will participate in an ongoing project, guided by the PI (Segal) and an experienced graduate student. The student will learn the principles of molecular dynamics simulations, mathematical modelling, script programming, high-performance computing, data analysis. The student will tackle one of the questions from above with simulations and modelling. The student will prepare a report (or a manuscript) on their work. The student will participate in group meetings and interact with other group members working on variety of problems in quantum and classical transport.

Qualifications: Curiosity, independence, persistence – with an interest in mathematical modelling and computational work. Prior programming experience *is not required* – join us and challenge yourself (and us)!



References:
[1] B. Gotsmann, A. Gemma, D. Segal,
Quantum phonon transport through channels and molecules: a perspective, [Applied Physics Letter 120, 160503 (2022).]

[2] J. J. Wang, J. Gong, A. J. H. McGaughey, D. Segal,
Simulations of Heat Transport in Single-Molecule Junctions: Investigations of the Thermal Diode Effect,
arXiv:2209.06266 J. Chem. Phys. 157 174105 (2022).