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CV/ biography

Evelyne Martin is Research Director at the ICube laboratory in Strasbourg. Her interest lies in the modeling of phenomena related to nanotechnologies by atomic-scale simulations. She is currently studying heat conduction at the nanoscale for applications in the thermal management of devices and for thermoelectricity. She is the main developer of the approach-to-equilibrium molecular dynamics (AEMD) methodology aimed at studying thermal transport on atomic trajectories substantially shorter than in earlier molecular dynamics methods. This approach was originally applied to silicon nanostructures described by interatomic potentials. AEMD is currently used to investigate heat propagation in amorphous materials and through molecular layers by resorting to first-principles molecular dynamics (DFT-based) simulations. Evelyne Martin has authored more than 50 articles in peer-reviewed international journals. She is currently coordinator of two ANR projects in the field of thermal properties.

Atomistic modeling of heat propagation in nanomaterials

In the present talk, I will report on the use of first-principles molecular dynamics (FPMD) to model heat propagation in nanomaterials. FPMD enables the calculation of atomic trajectories accounting for the electronic structure, obtained from density-functional theory (DFT). Therefore, FPMD can handle bonding situations quantitatively inaccessible to interatomic potentials, such as organic/inorganic interfaces or network-forming disordered materials. Despite the computational cost required by DFT, FPMD has been fruitfully applied to study thermal properties by resorting to the approach-to-equilibrium molecular dynamics (AEMD) strategy[1]. AEMD aims at studying thermal transport by exploiting affordable time trajectories corresponding to transient regimes. After a presentation of the methodology, I will focus on two applications. The first one is an interfacial molecular layer in between heat reservoirs. The thermal resistance of the layer is obtained under the verified assumption that the heat transport is driven by the transfer at the interface. The thermal resistance has two contributions, the first one corresponding to the bond between the molecules and the reservoirs, and the second attributed to heat conduction in the diffusive regime along the molecular chains[2]. Then, I will consider amorphous materials and the search for propagative modes in these systems. To this purpose, the thermal conductivity of two glasses, $GeTe_4$[3] and $Ge_2Sb_2Te_5$[4] (a standard material for non-volatile phase-change memories), has been determined as a function of the length in the direction of the heat transport. Our results are substantiated by an extrapolation at large sizes in quantitative agreement with experiments. The length dependence is a compelling evidence of the existence of propagative modes, expected to extend up to 30-50 nm, well above extended range order. Our results have profound implications on the reduction of thermal conductivity at the nanoscale and the thermal management of relevant devices.

[1]E. Lampin et al, J. Appl. Phys. 114, 033525 (2013) ;[2]T.-Q. Duong et al, J. Chem. Phys. 153, 074704 (2020) ; [3]T.-Q. Duong et al, soumis à J. Phys. Chem. Lett.; [4]T.-Q. Duong et al, Phys. Rev. Mat. 3, 105401 (2019)

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