ON THE ENHANCED THERMAL TRANSPORT PROPERTIES OF GRAPHENE NANOFLUIDS

Francesca Costanzo[1], Bernd Ensing[1,2] and Pablo Ordejón[1]

[1]*Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain*
[2] *Van't Hoff Institute for Molecular Sciences, University of Amsterdam, 1098 XH Amsterdam, The Netherlands*

Optimization of the thermal properties of fluids is important for storage and transport of heat in various sustainable energy applications. The dispersion of nanomaterials is an effective means to enhance the thermal properties of fluids, although the mechanism behind the enhancement remains thus far mysterious. Initially prompted by the interest of Abengoa Research (a company based in Spain, leader in research in the area of renewable energies) we use DFT calculations and molecular dynamics simulations to unravel how the heat capacity and the thermal conductivity of organic solvents are affected by dispersed graphene nanoflakes.

In this talk, I will show some preliminary results on how the size, the shape and the concentration of the nanoparticles affect the specific heat capacity and the thermal conductivity of the nanofluids. Several mechanisms to explain the enhancement are discussed, such as DMF layering onto the nanoflakes and graphene acting as accelerating centers for thermal waves.