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Thermal properties of graphene nanoflakes dispersed in DMF: A classical MD study including QM corrections

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Ionic liquids are one of the preferred options used by the industry for the storage of thermal energy in solar energy plants. Improving their thermophysical properties is an important goal to achieve more efficient heat storage and transportation media. A promising approach for improving these properties is to introduce nanoparticles dispersed in the ionic liquid or the molten salt, the so-called nanofluids. However, how thermophysical properties such as the heat capacity, self-diffusion, or heat conductivity depend on the microstructure of the nanofluids is still rather unknown. Molecular simulation, therefore, can play a major role in this research, as producing reliable experimental data for these systems is difficult and expensive. We have calculated by classical molecular dynamic simulations, thermal properties of disk-like graphene nanoflakes dispersed in organic solvent. In my contribution, I will discuss how the heat capacity and the thermal conductivity depend on the shape, the size and the density of the dispersed carbon nanoflakes. While thermal conductivity is well simulated by our classical model, the insertion of quantum corrections (QM) is necessary to calculate the heat capacity in good agreement with experiments. With our classical model including QM corrections, we are able to shed light and gather basic understanding on the dependence of thermal transport properties on the nature of solute-solute and solute-solvent interaction.

Biography

Francesca Costanzo has completed her PhD research at the University of Bologna, in 2000 with a thesis entitled: "Modified electrodes by conducting polymers". Since her PhD, she combined her experimental experience with the theoretical work at different levels of approximation in the fields of solid state physics and condensed matter. Her competence in ab initio MD simulation allowed her to model, for example, the interaction of molecules on carbon materials (graphene, single and double walled nanotubes, fullerenes), and water splitting chemistry on transition metal oxide surfaces. She acquired her computational knowledge working at prestigious universities and institutions in Cambridge, Leiden, Padua and Barcelona. Her output includes 30 scientific articles, many invited talks and oral presentations.

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