Séminaire du CETHIL

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Amphithéâtre Claude-Chappe

Thermal Transport across Organic-Inorganic Interfaces

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Résumé du séminaire

A self-assembled monolayer (SAM) junction is a periodic monolayer of organic molecules that bridges two metallic or semiconducting contacts. A nanocrystal array (NCA) is a periodic, three-dimensional array of metallic or semiconducting nanoparticles decorated with organic molecules. The electronic structure of these low-cost organic-inorganic hybrid materials can be carefully tuned, making them attractive alternatives to semiconductors in thermoelectric, photovoltaic, and electronic applications. While the electronic properties of SAM junctions and NCAs have been extensively studied, their thermal properties have received less attention.

To address this knowledge gap, we use molecular dynamics simulations and lattice dynamics calculations to predict the thermal conductance of SAM junctions of the thermal conductivities of NCAs. The modeling predictions are directly compared to experimental measurements. For the SAM junction, we resolve a long-standing discrepancy between measurements and predictions by considering the imperfect contact due to surface roughness. We find that the degree of vibrational overlap between the two contacts can be used to tune the junction thermal conductance. For the NCA, we examine the effects of nanoparticle size and composition on thermal conductivity. The organic-inorganic interfaces are found to be an important source of thermal resistance.

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