工学系研究科専攻間横断型教育プログラム
「機械システム・イノベーション」

GMSI

最先端融合科学イノベーション
教育研究コンソーシアム

東京大学 THE UNIVERSITY OF TOKYO

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Thermal Transport in Large Unit Cell Crystals

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Abstract:

In this seminar, I will describe how atomistic simulations and calculations can be used to predict and interpret the thermal transport properties of crystalline C_{60}, superatomic crystals, and metal organic frameworks. Thermal energy transport is dominated by atomic vibrations in these crystalline materials, which have unit cells that contain tens or hundreds of atoms. As a result of the large unit cells, transport physics emerge that are not present in small unit cell crystals such as silicon.

Molecular dynamics simulations are performed on the C_{60} crystal with (i) all degrees of freedom active, (ii) rigid cages that can translate and rotate, and (iii) a reduced-order point-mass model. The results allow for resolution of the effects of different types of degrees of freedom (intramolecular vibrations, intermolecular vibrations, and rotations) on thermal transport

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The superatomic crystals considered are periodic, three-dimensional arrays of C_{60} and Co_6X_8 ($PEt_3)_6$ (X=S, Se, Te) molecules. The electronic structure of these low-cost organic-inorganic hybrid materials can be carefully tuned, making them attractive alternatives to traditional semiconductors in thermoelectric, photovoltaic, and electronic applications. Small changes in the constituent molecules are found to have a pronounced effect on thermal conductivity. Regimes typical of crystalline and amorphous materials are observed and interpreted based on the rotational order/disorder of the C_{60} molecules.

MOFs are organic-inorganic hybrid material that contains Angstrom-sized pores and channels. They have application in gas storage, gas separation, and catalysis. By performing molecular dynamics simulations, the effects of pore size, shape, and filling gases on MOF thermal conductivity are predicted. The coupled mass and heat transfer across a MOF-gas interface is analyzed.

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