INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Friday, 19 May, 1:00 p.m.
Room IC 02-718

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Reverse non-equilibrium molecular dynamics simulations of silicon phononic crystals

Phononic crystals are periodically structured, synthetic materials that allow control of the propagation of elastic waves. Through the choice of the parameters of the periodic structuring opens the phonon dispersion relations can be modified and vibrational band gaps can be created. Phononic crystals have numerous potential applications in areas such as noise control, ultrasound imaging and telecommunications. Since the principal carriers of heat in non-metallic materials are phonons, nanoscale phononic crystals with operating frequencies in the THz regime can be utilized to control the flow of heat. This has potential applications in energy harvesting and novel heating or cooling technologies.

In this work, molecular dynamics simulations are used to study the thermal transport properties of silicon phononic crystals. The thermal conductance of the model systems is determined with the help of Reverse Non-Equilibrium Molecular Dynamics (RNEMD). RNEMD is a straightforward method for the determination of thermal conductances. The method has, however, some drawbacks that will be discussed. Results will be shown for the length dependence of the thermal conductance of the phononic crystals.