Nanoscale Heat Energy Transport: A Computational Study

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The application of nano devices has highlighted the need for greater quantitative understanding of materials at the nanoscale. Understanding the physics of such systems by computational study is particularly important, because their small size makes it is challenging to apply standard experimental measurement methods. Over the past decades advances in computer science have spurred advances in fundamental theoretical techniques, mathematical modelling, and numerical simulation, giving rise to a revolution with extraordinary impact for nanoscience and nanoengineering.

In this talk I will provide an introduction for both theorists and experimentalists to the molecular dynamics (MD) simulations and then looking at the applications of nano structures in associated research topics. MD simulation is an extremely powerful tool to handle many-body problems at atomic level, which numerically solves Newton's equation of motion for a many-body system. It has the advantage of simulating realistic material with accurate many-body interatomic interaction. In the context of thermal transport, MD simulation is a statistical mechanics approach, which relates the microscopic behavior in a system with its thermodynamics. According to statistical mechanics, physical quantities can be evaluated by averaging over configurations distributed according to a certain statistical ensemble.

References

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