Ab-initio thermal conductivity

A talk by Georg Madsen

Institute of Materials Chemistry, Vienna University of Technology

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Predictive modeling of the thermal transport in modern semi-conductor architectures is an inherently multi-scale problem. It requires the quantification of phonon scattering caused by various types of defects e.g. vacancies, interfaces and dislocations. However the modeling of thermal conductivity is based often on 50 year old analytical approximations, whose simplicity was driven by practical limitations rather than physical insight. I will introduce the ab-initio calculation of bulk thermal conductivity based on the Boltzmann transport equation. Starting from approximate and full calculations of the three phonon scattering rate the calculation of thermal conductivity for bulk materials will be introduced. The recently implemented Green's function approach for the calculation of the scattering rates for specific defects will then be introduced and exemplified.