O.32 Phonon-limited transport properties with ABINIT

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First-principles calculations of phonon-limited transport properties, such as conductivity, carrier mobility and Seebeck coefficient, represent an active area of research within the ab-initio community [1,2].

In this contribution, I will briefly review the different theoretical approaches commonly used to compute transport properties with particular emphasis on the linearized Boltzmann transport equation. Finally, I will discuss some technical aspects related to the ABINIT implementation.



^[1] Feliciano Giustino. Electron-phonon interactions from first principles. Rev. Mod. Phys. 89, 015003 (2017).

^[2] Samuel Poncé et al First-principles calculations of charge carrier mobility and conductivity in bulk semiconductors and two-dimensional materials. Reports on Progress in Physics 83, 036501 (2020).