COMPUTING THE INTRINSIC MOBILITY OF ELECTRONS ANS HOLES IN SEMICONDUCTORS

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Computing the electronic transport from first principles is crucial for the discovery and development of new functional materials. Recently, different works have reported the *ab initio* phonon-limited mobility for various semiconductors and metals [1, 2].
We report the new developments for the ABINIT package to compute the electron self-energy due to electron-phonon coupling using a plane-wave basis set. In particular we focus on computing the lifetimes from the imaginary part of the self-energy at the Kohn-Sham energies, which we use to solve the linearized Boltzmann transport equation and obtain the phonon-limited mobility in a single ABINIT run.
In the first part of the talk we will present convergence studies for the mobility of Si and GaP and introduce different techniques used to speed up the computations and reduce the memory requirements. In the second part we will discuss technical aspects of the implementation of these techniques. These include the interpolation of the DFPT potentials, the use of symmetries, check point and restart, the tetrahedron integration, double-grid and filtering. We will finalize by outlining problems encountered during development as well as our suggested solutions.

References

[1] S. Poncé, E. R. Margine, F. Giustino Phys. Rev. B **97**, 121201(R) (2018)

[2] J. I. Mustafa, M. Bernardi, J. B. Neaton, S. G. Louie, Phys. Rev. B **94**, 155105 (2016).