Ab initio calculations of electronic transport properties and of the thermoelectric phonon drag effect in semiconductors

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Résumé

In the present work, we first consider the state-of-the-art computational techniques to accurately
calculate the electronic transport properties of n-doped silicon. The calculations, performed with the
EPW code [1], are based on the iterative solution of the linearized Boltzmann transport equation (BTE)
coupled to the data obtained using density functional theory and density functional perturbation theory.
Concurrently, a special focus is made on understanding the enhancement of the Seebeck coefficient by
electron-phonon coupling, known as the "phonon-drag" effect [2]. To take this effect into account, we
modified the standard EPW code so that it allows us to solve the BTE for electronic transport in
presence of non-equilibrium phonon populations introduced by a temperature gradient. We will present
our recent results related to electron-phonon scattering times, phonon and/or impurity limited carrier
mobility, as well as the Seebeck coefficient of silicon. Our results for n-doped silicon not only show a
good agreement with the experimental data [3] but also pave the way to further understand the
contribution of phonon-drag in semiconductor nanostructures, which still remains largely unexplored. **References**
1) S. Poncé, E. R. Margine, C. Verdi, and F. Giustino, Comput. Phys. Commun. 209, 116 (2016).
2) C. Herring, Phys. Rev. 96, 1163 (1954).
3) T. H. Geballe and G.W. Hull, Phys. Rev. 98, 940 (1955).

Mots-Clés: Density functional theory, electronic transport, Seebeck, Phonon, drag

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