ELPHBOLT - A FREE SOFTWARE FOR COUPLED ELECTRON-PHONON BOLTZMANN TRANSPORT

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Accurate, parameters-free prediction of the electronic and phononic transport properties of real materials is crucial for understanding the underlying non-equilibrium physics and for identifying candidate materials for applications. In the typical approach, when the transport of one species is calculated, the other species is assumed to remain in equilibrium; i.e. the "drag effect" is ignored. It is, however, known that in certain cases the drag effect dominates the transport phenomena. We present here the Free/Libre elphbolt code which can efficiently compute the electronic and phononic transport properties using a self-consistent, *ab initio* solution of the coupled Boltzmann transport equations of the two systems. A schematic of the elphbolt workflow is shown in Figure 1.

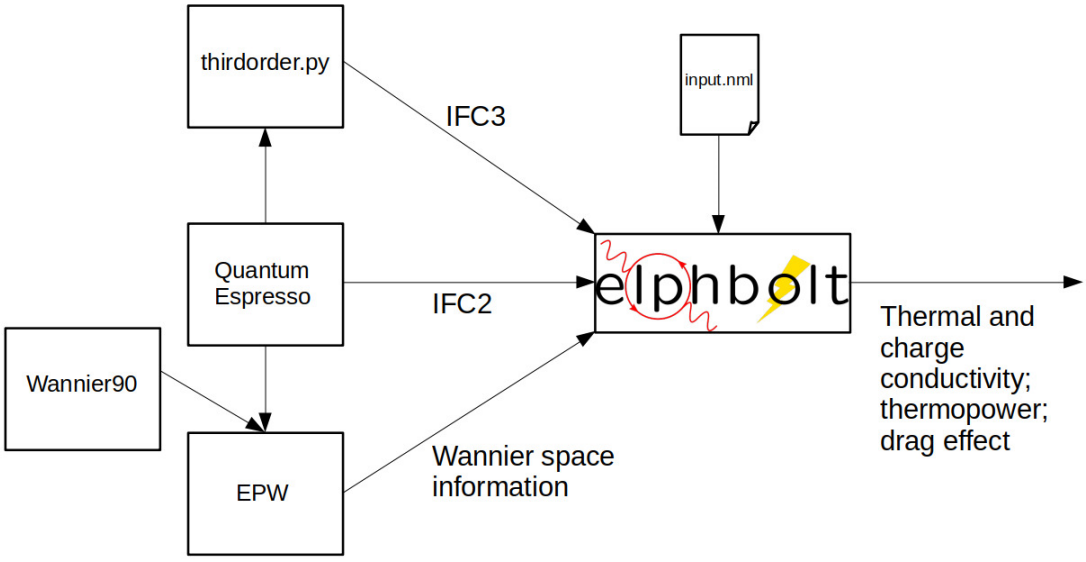

Figure 1. The elphbolt workflow. Real space information such as the 2nd and 3rd order force constants (IFC2 and IFC3, respectively), Wannier representations of the electronic Hamiltonian, electron-phonon interaction vertex, etc. are read from the publicly available softwares on the left. Elphbolt then computes the transport coefficients on the right following the instructions from the user.

Keywords
Drag effect, electron, phonon, Boltzmann transport.

Reference(s)

[1] N.H. Protik, Ch. Li, M. Pruneda, D. Broido, P. Ordejón. "elphbolt: An *ab initio* solver for the coupled electron-phonon Boltzmann transport equations", arXiv preprint arXiv:2109.08547 (2021).