Quantum ESPRESSO: from density-functional theory to dual wave-particle transport and device simulation

Michele Simoncelli
Theory of Condensed Matter Group of the Cavendish Laboratory, University of Cambridge (UK)

ABSTRACT

Understanding and quantitatively predicting transport phenomena in solids, involving for example charge or heat, from first principles is crucial to design devices for energy conversion or management. In general, the functioning of these devices is governed by an interplay between microscopic, intrinsic materials' properties (determined by the atomistic structure and composition) and macroscopic device properties (such as shape and boundary conditions). We present recent advances in Quantum ESPRESSO, an open-source density-functional-theory (DFT) software, that are relevant for the bottom-up, multiscale simulation of devices. First, we discuss how to compute from DFT all the parameters entering in the microscopic Wigner formulation for transport in solids. This formulation encompasses the emergence and coexistence of particle-like and wave-like conduction mechanisms, enabling quantitative predictions for the intrinsic thermal (electrical) conductivity of solids ranging from crystals to glasses (semiconductors to metals). We then discuss how this microscopic formulation can be coarse-grained into continuum models that describe, at a reduced computational cost, how the shape and size of the device affect transport. Finally, we show that these continuum models can be parameterized from DFT, and rationalize non-diffusive, viscous transport phenomena recently observed in devices made of layered materials.

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