MS-DFT: Quantum transport from a multi-space excitation viewpoint

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ABSTRACT

For the simulation of non-equilibrium open junction systems under finite bias in a first-principles manner, there exist several motivations to seek an alternative to the standard approach of combining density functional theory (DFT) and nonequilibrium Green's function (NEGF) formalisms. For example, for graphene electrode-based van der Waals 2D tunneling transistors, *ab initio* simulations are currently not possible due to the inherent limitations of the DFT-NEGF method [1-2]. In this presentation, I will discuss the formulation and applications of the multi-space constrained-search DFT (MS-DFT) that we have been developing at KAIST for the past decade plus [1-4]. Seeking an alternative to the standard Landauer picture for quantum transport, we first propose a viewpoint that maps quantum transport processes to space-resolved (drain-to-source) optical excitation counterparts. The multi-space excitation picture for quantum transport then allows the formulation of microcanonical approaches for quantum transport, and the resulting MS-DFT provides unique opportunities in understanding and designing nanoscale devices such as the graphene-based 2D tunneling transistor in operando conditions. Importantly, unlike in the grand-canonical DFT-NEGF, the non-equilibrium total energy as well as quasi-Fermi levels and voltage drop profile can be obtained within the microcanonical MS-DFT [3,4]. Several extensions and applications of MS-DFT will be also outlined.

REFERENCES

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