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Quantum-hybridization negative differential resistance from halide perovskite nanowires and vertical graphene junctions

In the effort to develop advanced electronic, optoelectronic, energy, and bio devices based on emerging low-dimensional materials, first-principles or *ab initio* simulations are playing an increasingly important role by providing atomistic information that are not easily accessible in experiments. For this purpose, a key ingredient that is still relatively immature and should be further developed is the capability to treat non-equilibrium open junction systems under finite bias in a first-principles manner. In this talk, I will first apply the existing machinery that combines density functional theory (DFT) and nonequilibrium Green's function (NEGF) formalisms and predict that ultrahigh negative differential resistance (NDR) can be obtained from the nanowires derived from recently synthesized one-dimensional (1D) halide perovskites [1]. Next, I will discuss the limitations of DFT-NEGF in simulating the finite-bias nonequilibrium electronic structure in nanoscale junctions and introduce the novel multi-space constrained search DFT (MS-DFT) formalism that we have recently developed. The MS-DFT formulation goes beyond the standard DFT-NEGF in several aspects, and as an application example I will consider graphene-based two-dimensional (2D) vertical heterosturcture tunneling transistors, which show NDR and are a promising platform to realize next-generation "More Moore" and "More than Moore" devices [2]. It will be emphasized that in both cases NDR arises from the novel "quantum-hybridization" NDR mechanism (Fig. 1).

References

[1] M. E. Khan, J. Lee, S. Byeon, and Y.-H. Kim, Adv. Funct. Mater. (2019) DOI: 10.1002/adfm.201807620).
[2] H. S. Kim and Y.-H. Kim (2018) arXiv:1808.03608 [cond-mat.mes-hall].

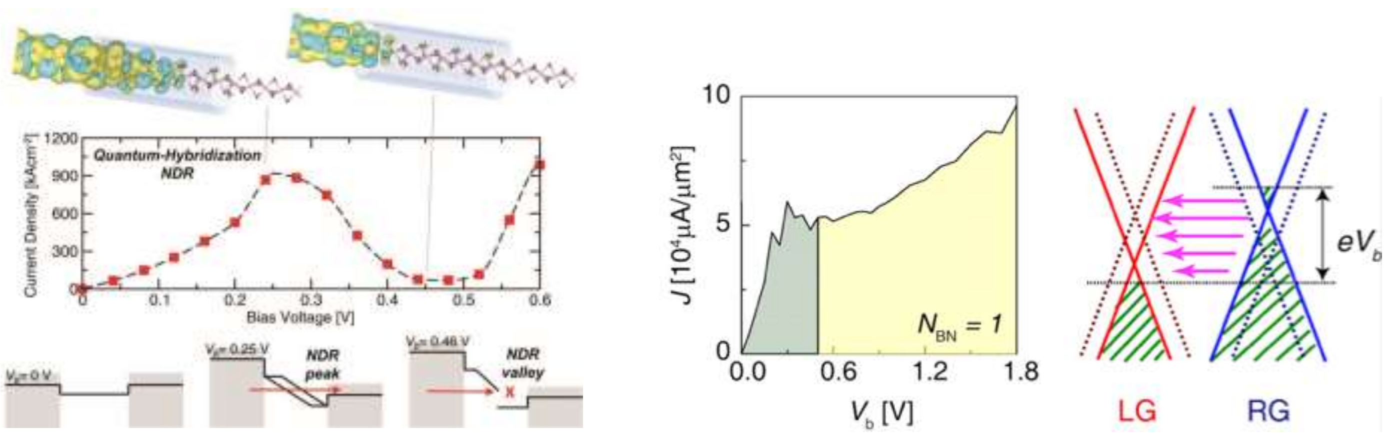

Figure 1: Quantum-hybridization NDR from 1D halide perovskite nanowires [1] (left) and graphene electrode-based 2D vertical tunneling transistors [2] (right).