Unconventional Current Scaling and Edge Effects for Charge Transport through Molecular Clusters

Metal-molecule-metal junctions are the key components of molecular electronics circuits. Gaining a microscopic understanding of their conducting properties is central to advancing the field. In the present contribution we highlight the fundamental differences between single-molecule and ensemble junctions focusing on the fundamentals of transport through molecular clusters. In this way, we elucidate the collective behavior of parallel molecular wires, bridging the gap between single molecule and large-area monolayer electronics, where even in the latter case transport is usually dominated by finite-size islands. On the basis of first-principles charge-transport simulations, we explain why the scaling of the conductivity of a junction has to be highly non-linear in the number of molecules it contains. Moreover, transport through molecular clusters is found to be highly inhomogeneous with pronounced edge effects determined by molecules in locally different electrostatic environments. These effects are most pronounced for comparably small clusters, but electrostatic considerations show that they prevail also for more extended systems.

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