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Understanding Molecular Conduction: Old Wine in a New Bottle?[1]

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Molecules provide an opportunity to test our understanding of fundamental non-equilibrium transport processes, as well as explore new device possibilities. We have developed a unified approach to nanoscale conduction, coupling bandstructure and electrostatics of the channel and contacts with a quantum kinetic theory of current flow. This allows us to describe molecular conduction at various levels of detail, – from quantum corrected compact models, to semi-empirical models for quick physical insights, and 'first-principles' calculations of current-voltage (I-V) characteristics with no adjustable parameters. Using this suite of tools, we can quantitatively explain various experimental I-Vs, including complex reconstructed silicon substrates. We find that conduction in most molecules is contact dominated, and limited by fundamental electrostatic and thermodynamic restrictions quite analogous to those faced by the silicon industry, barring a few interesting exceptions. The distinction between molecular and silicon electronics must therefore be probed at a more fundamental level. Ultra-short molecules are unique in that they possess large Coulomb energies as well as anomalous vibronic couplings with current flow – in other words, strong non-equilibrium electron-electron and electron-phonon correlations. These effects yield prominent experimental signatures, but require a completely different modeling approach – in fact, popular approaches to include correlation typically do not work for non-equilibrium. Molecules exhibit rich physics, including the ability to function both as weakly interacting current conduits (quantum wires) as well as strongly correlated charge storage centers (quantum dots). Theoretical treatment of the intermediate coupling regime is particularly challenging, with a large 'fine structure constant' for transport that negates orthodox theories of Coulomb Blockade and phonon-assisted tunneling. It is in this regime that the scientific and technological merits of molecular conductors may need to be explored. For instance, the tunable quantum coupling of current flow in silicon transistors with engineered molecular scatterers could lead to devices that operate on completely novel principles.

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