Orbital theories for molecular electronic devices

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Ballistic electron transport through molecules occurs, for instance, in molecular electronic devices (MEDs). In MEDs, two external contacts are connected to a molecule and the current is measured as a function of the applied voltage. Ballistic transport is characterized by the absence of coupling between electronic and nuclear degrees of freedom so that the coherence of the electronic wave function is preserved across the molecule. Theories of MEDs are quite involved in general, requiring advanced Green's function techniques. However, various prominent features of MEDs can be understood drawing only on elementary quantum theory. To support this point of view, we discuss simple models [1-4] which enable one to reproduce and predict key features of MEDs. We present, for example, a two component orbital theory. In this theory, the device orbitals (DOs) are written as a two component wave function, each of which is much simpler to construct than the combined orbital. Using these DOs, the conductance can be calculated drawing on the source-sink potential approach [1]. To illustrate our theory, we apply it to explain the conductance suppression in cross-conjugated systems and the dependence of the conductance on the contact position in aromatic systems. Furthermore, we apply our models to analyze the conductance of finite graphene flakes of varying shapes and sizes. We establishing simple concepts relating the structure of the graphene flakes to their conductance.

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