Ab initio computations of stability, electronic structure and transport properties of molecular junctions - a review

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Molecular junctions are widely considered as the basic structural units in molecular electronics. Unlike the traditional devices of the silicon industry the transport phenomena in molecular junctions can be substantially influenced by the interference effects and Coulomb correlations. For the given molecule bridging the leads, the current-voltage characteristic of a junction can vary considerably with the details of atomic arrangements at and near the bonding place.

In order to obtain a realistic description of the electronic transport through the junction the *ab initio* approach are usually applied. However, most of existing computations overestimate the electric current, often by order of magnitude or more. In this talk the efforts to compute the stable configuration of the junction as well as the electric current will be reviewed and the possible reasons of quantitative disagreement between the experiment and *ab initio* theory will be discussed.

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