Electronic transport in molecular nanodevices from *ab-initio* calculations

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Abstract

The striking development achieved in the process of fabricating devices of molecular size has promoted the birth of what is now termed *Molecular Electronics*, where just a few molecules (or even a single one) become the key part of an electronic circuit. However, the experimental conditions are such that, frequently, the atomistic realization of these *molecular nanodevices*, decisive for their understanding and improvement, is difficult to ascertain from the experiments, thus making theoretical evaluation of electronic transport a valuable aid. Here, the link between transport properties and structural/electronic details of molecular nanodevices is stressed by applying the *ab-initio* theoretical approach implemented in the so-called *Gaussian Embedded Cluster Method* [1] on several examples.

References

[1] J. J. Palacios, A. J. Pérez-Jiménez, E. Louis, E. San-Fabián, J. A. Vergés, Y. García, *Molecular electronics with GAUSSIAN98/03*, in *Computational Chemistry: Reviews of Current Trends*, Vol. 9, edited by J. Leszczynski (World Scientific, Singapore, 2005).