Conductance of a hydrogen molecule: an ab initio study

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Present trends in the miniaturization of electronic devices suggest that ultimately single molecules may be used as electronically active elements in a variety of applications. Recent advances in the manipulation of single molecules now permit to contact an individual molecule between two electrodes and measure its electronic transport properties. In a recent experiment Smit at al. [1] have measured the conductance of a single H_2 molecule forming a stable bridge between Pt electrodes. In contrast to results for other organic molecules, the bridge has a nearly perfect conductance of one quantum unit, carried by a single channel.

In this work we present a theoretical analysis of this experiment using a combination of ab initio quantum chemistry calculations and non-equilibrium Green functions techniques [2]. This approach allows us to show how the conduction channels arise from the molecular orbitals and elucidate which specific properties of the individual orbitals determine their contribution to the current. In the case of the hydrogen molecule we demonstrate that the current flows through the 1s level of hydrogen, resulting in a single conduction channel. Thus, the molecule limits the number of available channels, as compared to the five of a single-atom Pt contact, thereby acting as an effective *channel filter*. This constitutes an ideal example of how a single molecular level controls the macroscopic current through a single-molecule junction.

[1] R.H.M. Smit, Y. Noat, C. Untiedt, N.D. Lang, M. van Hemert, and J.M. van Ruitenbeek, cond-mat/0208407.

[2] J. Heurich, J.C. Cuevas, W. Wenzel and G. Schön, Phys. Rev. Lett. **88**, 256803 (2002).