Doping metallic chemically active nanocontacts: Platinum and Gold in a Hydrogen environment.

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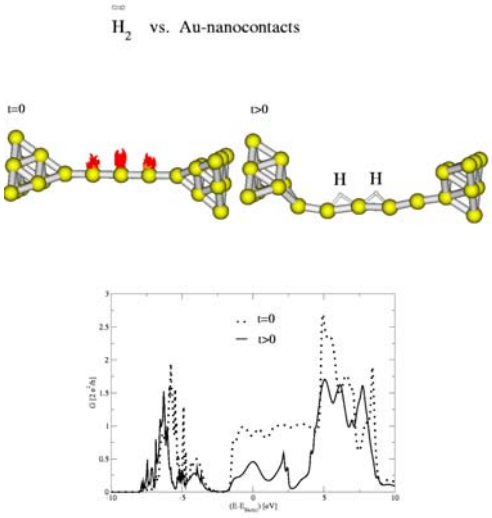
We show the state-of-the-art first-principles methods developed by our group to study electronic transport in nanobridged metallic systems[1, 2]. These dimension-reduced junctions are the focus of growing attention of experimental and theoretical groups, mainly due to practical applications and discrepancies between theoretical results[3–7]. Up to this point, discussion is centered around three points:

- How does the nuclear configurations at the nanocontact affect the electronic transport?
- What are the intrinsic limitations of standard quantum chemistry tools, mainly Density Functional Theory, for this particular application?
- Do incoherent events influence the process of electronic transport?

Our studies intend to give quantitative answers to these questions.

The process of **formation of nanocontacts** is shown as a *mechanical* way to **induce catalityc activity**. We apply methods established by quantum chemistry to study/predict chemical reactions of finite systems to our *infinite* metallic nanocontacts. Models assuming the existence of energetically well-defined molecular orbitals are employed throughout the analysis of the density of states in the zone to be chemically studied. Also within this context we begin to explain electronic transport in molecular/atomic bridged systems. **Atoms/Molecules** are presented **as dopants on metallic nanocontacts**[8, 9]. Numerical results are obtained and discussed in correspondence to recent experimental results for Platinum and Gold nanocontacts made in a Hydrogen environment[4, 5, 7, 9].

FIG. 1: Conductance as a function of energy (referred to the Fermi energy) for the clusters shown as $t = 0$ and $t > 0$.



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