

Last advances in single-molecule electric contacts

Ismael Díez-Pérez, Josh Hihath, Thomas Hines, Zhihai Li, Nongjian Tao

Institute for Bioengineering of Catalonia, Baldori Reixac 1-5, Barcelona 08028, Spain
Biodesign Institute at Arizona State University, 1001 S. McAllister Ave., Tempe, AZ85287, USA

idiezper@asu.edu, idiez@ibecbarcelona.eu

During the last decade, the first experimental demonstrations of the feasibility to build single-molecule electric contacts [1,2] have led to a huge revolution in the field of Molecular Electronics. The possibility to study charge transport through a single molecule bridged between two macroscopic metal beads has placed this field in an unbeatable position to directly address fundamental questions on the relation between the molecular structure and the charge transport behavior. For example, it has already been described the impact that the presence of certain chemical groups in the single-molecule contact, such as saturated linear chains [3], conjugated blocks [4], electron donor/acceptor groups [5] or redox centers, has in the dominating charge transport mechanism.

In this contribution, we describe our latest advances toward the fundamental understanding of the main parameters dominating the charge transport through organic scaffolds and we demonstrate how the chemical structure can be tailored to achieve a desired electron transport profile in the single-molecule device. In the first part, we will describe the last implemented technical methodologies to univocally identify when a single-molecule contact is formed between two metal electrodes. The methodologies are based on the introduction of small AC perturbations within the electrode-electrode gap separation and the corresponding AC current response detection in the frequency space [6,7]. Together with the AC methods, long pulling programs applied to the molecular contact are also performed at the end of the experiment as a method to evidence the single-molecule nature of the junction. After this technical description, two examples showing how to tailor the single-molecule electron transport through the molecular design will be presented. The first case presents one of the first examples of rectification behavior (diode effect) in a single-molecule device [8]. Here we demonstrate that it is possible to go from a perfectly symmetric to a highly rectifying charge transport behavior by introducing small chemical modifications within the molecular architecture (see Figure 1).

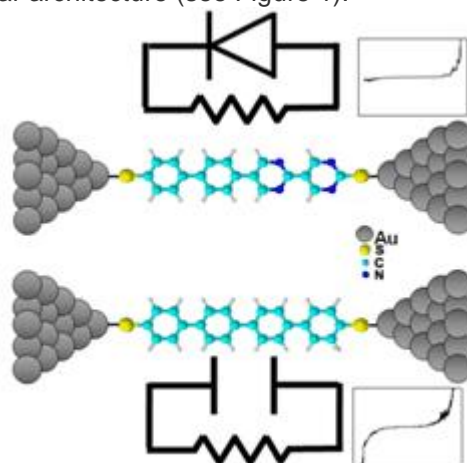


Figure 1: Representation of two single-molecule devices with similar polyphenyl molecular blocks displaying symmetric (bottom) and diode (top) charge transport behaviors.

The second case explores the feasibility to design single-molecule field effect transistors (FET) by using a graphene-like molecular structure (coronene derivatives) through the exploitation of the previously introduced electrochemical gate [9] (see Figure 2) in order to modulate the conductance of the single-molecule contact and control the ON-OFF behavior as in conventional FET setups [10]. This last example opens up a bottom-up approach for the future design of functional FET based on graphene materials. The final part of this paper will describe another example of how to modulate the single-molecule conductance in this case by using a mechanical perturbation. This last presented device constitutes the first demonstration of single-molecule electromechanical effect [7].

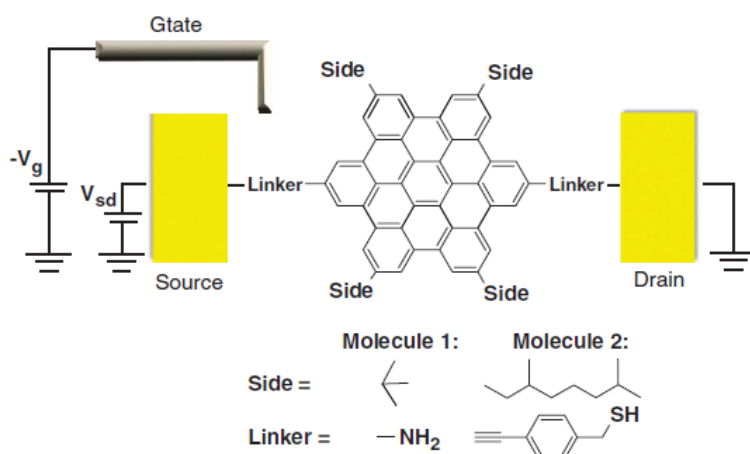


Figure 2: Representation of a single-molecule FET built with coronene derivatives and gated with a reference electrode in an electrochemical configuration.

References

- [1] M. A. Reed, C. Zhou, C. J. Muller, T. P. Burgin, J. M. Tour *Science* **278** (1997) 252.
- [2] B. Q. Xu and N.J. Tao *Science* **301** (2003) 1221.
- [3] X. Li, J. He, J. Hihath, B. Xu, S. M. Lindsay, N.J. Tao *JACS* **128** (2006) 2135.
- [4] L. Venkataraman, J. Klare, C. Nuckols, M. S. Hybertsen, M. Steigerwald *Nature* **442** (2006) 904.
- [5] L. Venkataraman, Y. S. Park, A. C. Whalley, C. Nuckolls, M. S. Hybertsen, M. Steigerwald *Nano Letters* **7** (2007) 502.
- [6] J. Xia, I. Díez-Pérez, N.J. Tao *Nano Letters* **8** (2008) 1960.
- [7] I. Diez-Perez, T. Hines, J. Hihath, Z.-S. Wang, G. Zhou, K. Müllen, N.J. Tao *Nature Nanotechnology*, accepted 2011.
- [8] I. Diez-Perez, J. Hihath, Y. Lee, L. Yu, L. Adamska, M. A. Kozhushner, I. Oleynik, N.J. Tao. *Nature Chemistry* **1** (2009) 635.
- [9] B. Q. Xu, X. Y. Xiao, X. M. Yang, L. Zang, N.J. Tao *JACS* **127** (2005) 2386.
- [10] I. Diez-Perez, Z. Li, J. Hihath, J. Li, C. Zhang, X. Yang, L. Zang, Y. Dai, X. Feng, K. Müllen, N.J. Tao *Nature Communication* **1** (2010) 31.