Graphene as a promising electrode for low current attenuation in molecular junctions

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Although technologically relevant molecular electronic devices still seem a long way off, the ability to measure the electrical properties of single molecules can be nowadays achieved with a variety of techniques. From these new measurements, there is an increasing realization that new single molecule electrical junction functionality can be achieved through the use of nonmetallic electrodes, with contacts such as carbon-based materials. It is then suggested that these materials have the potential to be valuable alternative electrode materials for molecular electronics in the next generation of nanostructured devices. Here, as a first step toward realizing the graphene potential as electrodes, we demonstrate its use as a bottom electrode in place of the more commonly used gold. The well-studied system of thiol-terminated alkane molecular bridges was selected as a test-bed to investigate the possibility to use graphene electrodes to form single molecule junctions. Combined STM measurements and Density Functional Theory associated to a Keldysh-Green formalism, reveal a strong reduction of the electronic length decay. This lower attenuation factor leads to higher junction conductance for the longest junctions studied here. This work suggests that novel nonmetallic 2D materials could serve as promising electrodes to construct nonsymmetric junctions with tunable attenuation factors.

References

- [1] Q. Zhang et al, Nano Letters, 16 (2016) 6534
- [2] C. González et al, Nanotechnology, 27 (2016) 105201
- [3] Y. J. Dappe *et al*, Nanoscale, 6 (2014) 6953



Figure 1: logarithmic plot of the conductance as a function of the number of CH2 groups. The red line represents the theoretical values, the black line is experimental data for Au-molecule-graphene junctions, and the blue line is the literature data for Au-molecule-Au junctions.