Theoretical study of carbon-based tips for Scanning Tunnelling Microscopy

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Abstract
Motivated by recent experiments, we present here a detailed theoretical analysis of the use of carbon-based conductive tips in Scanning Tunnelling Microscopy (STM). In particular, we employ ab initio methods based on density functional theory to explore both graphitic and diamond-like tips for imaging with a scanning tunneling microscope (STM), and we compare them with standard metallic tips made of gold. We investigate the performance of these tips in terms of the corrugation of the STM images acquired when scanning a single graphene sheet. Moreover, we analyse the impact of the tip-sample distance and show that it plays a fundamental role in the resolution and symmetry of the STM images. We also explore in depth how the adsorption of single atoms and molecules in the tip apexes modifies the STM images and demonstrate that, in general, it leads to an improved image resolution. Besides, we show that carbon tips can be combined with other carbon nanostructures, such as graphene, to form all-carbon molecular junctions with molecules like benzene or C_{60}. Our results show that the use of carbon tips can lead to relatively conductive molecular junctions. Finally, the ensemble of our results provides strong evidence that carbon-based tips can significantly improve the resolution of STM images, as compared to more standard metallic tips, which may open a new line of research in Scanning Tunnelling Microscopy.

References

Figures

Figure 1: (left) artistic representation of a graphene electrode based molecular junction. (right) Calculated STM image of a graphene plane obtained with our graphitic tip (placed at 4.5 Å), for a specific tip orientation related to the graphene layer, showing a honeycomb pattern.