Toward a real-time time STM simulation engine using Green's functions

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Within the framework of atomic resolution STM images, the understanding of relations between the surface, the tip, the adsorbate (if present) and the bulk materials is not always straightforward. Depending on the inherent quality of an experimental STM image, the nature of component within the entire system can be determined with a very limited certainty. In order to extirpate vital information from STM images, a strong coupling between experimental and theoretical analysis is always a source of success and should be strongly encouraged.

One common way to compare experimental images with theoretical one is to use the Tersoff-Hamann [1] model. Even if that model is very popular and effective, the absence of the tip contribution in the tip-surface interaction is nowadays a limiting factor. With the constant increase in computer power it is now feasible to simulate a part of the system from first principles --- for example using the density functional theory (DFT). Although DFT can address sophisticated systems with a very good accuracy, it cannot be reasonably used to perform large and non-periodic calculations where the computational time and the memory required become excessively demanding. Hence, a compromise between accuracy and time spent for atomistic calculations, such as for STM simulations, leads us to use a suitable approach such as tight-binding Hamiltonian in conjunction with Green's functions. Here, we followed the general computational approach developed by Cerdá *et al.* [2] that was implemented in the GREEN code. This code has been recently [3] improved with highly parallel subroutines. In addition, a more intimate coupling between GREEN and the quantum-mechanical software, SIESTA [4], allows a rapid and appropriate determination of atomic parameters needed for STM simulations. This opens perspectives for the development of new materials and a faster comprehension of STM images. We will show a few computing benchmarks with this package on large parallel machines showing its efficient scalability. We will also present a few representative test cases where a comparison to Tersoff-Hamann images was performed, and which were supported by density functional theory. A recent work [5] on multilayers of polythiphene on graphite and graphene (see Fig. 1) will emphasize the strength of our STM simulation approach to reveal properties related to charge transport and π-electron coupling.

References

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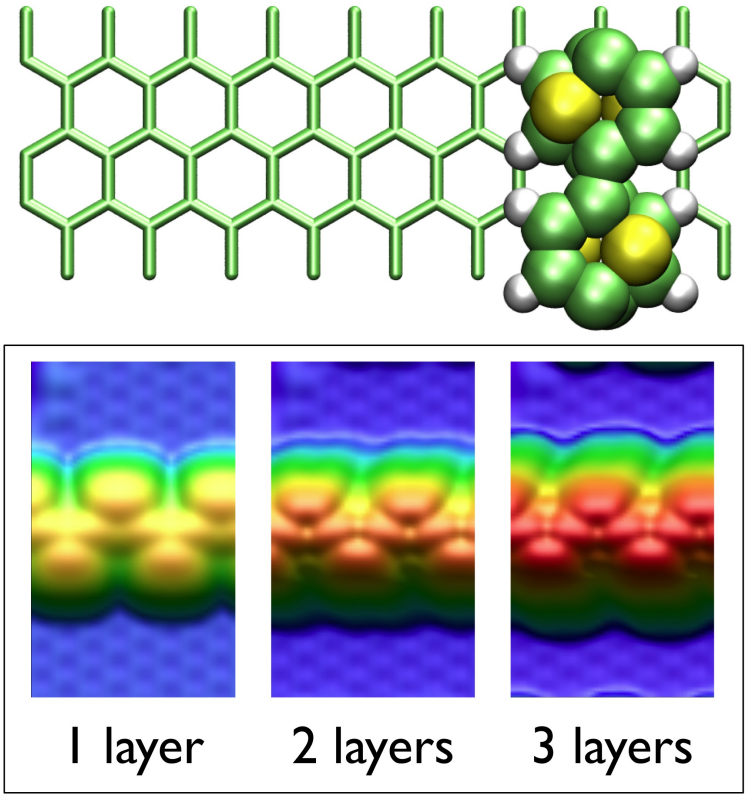
Figures



Molecular model of the unit cell considered for a polythiophene multilayer stack on graphite (upper panel) and resulting STM images calculated for one, two and three polythiophene layers on graphite (lower panel). (I = 0.1 nA, V = 1.5 V)