STM images and spectroscopy of molecules on metal surfaces: CP2K+XT/DFTB+XT open software suite

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We developed a theoretical and computational approach for simulations of STM images and spectroscopy, in particular of molecules on metal surfaces. We employed the DFT and DFTB based atomistic approach combined with the Green function technique [1], which offers a framework to consider a tip, molecule and surface as one integrated system and taking into account the tip geometry. Besides, it captures the interference [4] and interaction effects. This new computational approach can be applied for the investigation of finite-voltage effects and describe the higher molecular transport states We developed the DFTB+XT computational package [2], based on the DFTB+ source code [3]. It makes possible and convenient calculations for large-scale molecular nanosystems on metall surfaces. As an example, we consider the conjugated polymers composed of alternating donor and acceptor repeat units, namely, DPP-based molecules on the Au(111) surface, investigated experimentally by the group of F. Moresco. We work on the extension of the platform including the CP2K code to make available general DFT and semi-empirical Hamiltonians.

References

[1] D. A. Ryndyk, *Theory of quantum transport at nanoscale*, Springer, 2016.
[2] D. A. Ryndyk, *DFTB+XT open software package for quantum nanoscale modeling*; http://quantranspro.org/dftb+xt/.

Figures

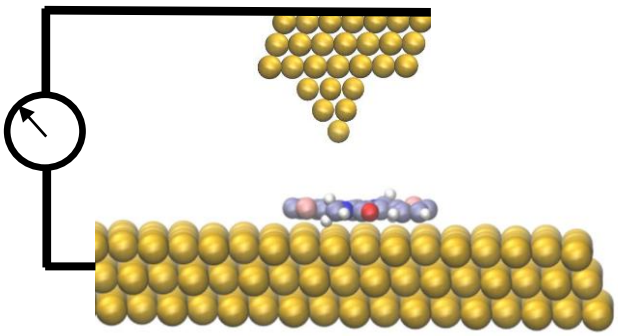

Figure 1: Schematic representation of the STM setup. Both substrate/molecule and tip are modelled atomistically.

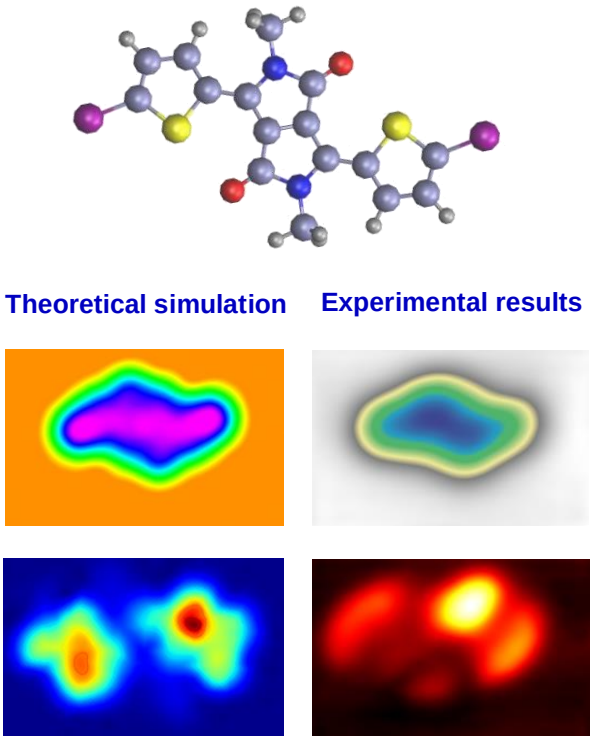

Figure 2: DPP on Au(111): STM image at small voltage (top) and dI/dV image of the LUMO.

[3] B. Aradi, B. Hourahine, Th. Frauenheim. J. Phys. Chem. A, **111** 5678 (2007). http://dftbplus.org/.
[4] P. Karasch, D.A. Ryndyk, Th. Frauenheim, Phys. Rev. B, arXiv 1802.00199 (2018).