Advancing scanning probe microscopy simulations: A decade of development in probe-particle models

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Since its inception more than a decade ago [1], the probe particle model has become an important tool for simulating high-resolution SPM images obtained with flexible tip apices, shedding light on the origin of the contrast patterns observed in experiments. Our recent review [2] discusses the development of the probe particle simulations over the years, with emphasis on the open source *ppafm* package for AFM simulations [3]. Starting from a simple model utilizing a Lennard-Jones force field, *ppafm* has expanded to include various force field models for electrostatic and Pauli interactions utilizing data from *ab initio* calculations, as well as other simulation modes including STM and KPFM. The recently implemented GPU acceleration has sped up the simulations by 2-3 orders of magnitude, enabling rapid generation of very large datasets, which has been instrumental in the development of machine learning tools for SPM image interpretation. Other recent enhancements to the package include better project structure, more documentation, and a graphical user interface, all making the package more user friendly and easier to approach.

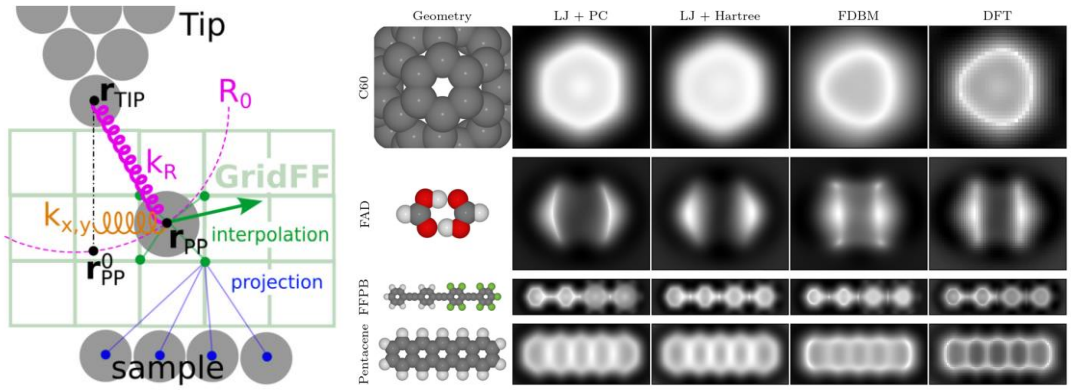

Figure 1. (left) Schematic of the probe particle simulation model. (right) *ppafm* simulations of various molecules using different force-field models with increasing level of accuracy and a comparison to DFT.

References:

[1] P. Hapala et al. Phys. Rev. B **90** (8), 085421 (2014).

[2] N. Oinonen, et al. Comput. Phys. Commun. **305,** 109341 (2024).

[3] ppafm repository: https://github.com/Probe-Particle/ppafm