Scanning Probe Microscopy: theory meets experiment

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Invention of Scanning Probe Microscopy enabled to image surfaces with atomic resolution. Further development converted SPM from imaging to a tool enabling control and modification at atomic scale. With advent of Atomic Force Microscopy, more often scanning procedure takes place in the near-to-the contact regime (see e.g. [1]). In this regime, the probe proximity strongly modifies the surface structure hindering the precise interpretation of experimental results. Further proliferation of Scanning Probe method is strongly dependent on the better understanding of undergoing processes during scanning processes.

Advanced theoretical analysis based on first principle DFT total energy methods combined with the transport calculations based on Green's function techniques [2] offers such possibility. We will discus key effects playing an important role during the formation of the atomic contact between tip and sample and the electron transport through the contact. The calculations allow to shed more light on factors playing an important role in atomic contact formation such as (i) a structural relaxation [3]; (ii) a modification of the electronic structure [4]; (iii) a collapse of the tunneling barrier [3]; (iv) the importance of elastic multiple-scattering processes of electrons [5]; and (v) modification of surface dipoles [6].

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