Probing the elastic response within a single molecule

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Controlled modification of atomic geometries in molecules and materials is an exciting goal for non-contact atomic force microscopy (NC-AFM), because various property changes like shifts of electronic energy gaps are expected. However, inducing and characterizing geometry changes from experimental tip-molecule interaction measurements constitutes a difficult goal already. This work thus aims at demonstrating controlled elongation with submolecular precision in a spring-like molecule and extracting the elastic response. A model system of nonahelicene ([9]H) and coronene (cor) was studied on Ag(110) and distance dependent interaction measurements (*Δf(z)* curves) were reproduced with an empirical model (Fig.1b). These show that cor behaves like a rigidly bound particle, whereas [9]H exhibits an elastic response. Probing the softest part of the backbone in [9]H yields then a spring constant of 6.1 Nm^{-1}. The structures of the tip and molecule are retained between 1D curve measurements. This permits a tip position dependent study above [9]H (Fig.1a), allowing the acquisition of 3D-AFM data. The analysis with the presented model reveals a strong anisotropic response with respect to the tip position (Fig.1c), which hints at special intramolecular interactions in [9]H. Different degrees of aromaticity rationalize the observation and establish the relevance of quantum effects in molecular elasticity measurements with lateral resolution.

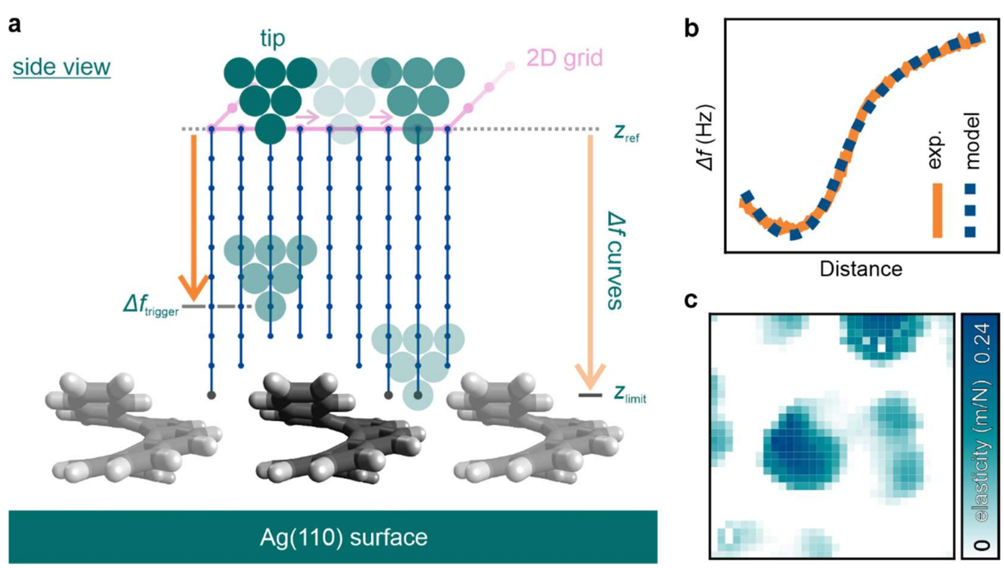

Figure 1. a Schematic of 3D-AFM data acquisition protocol where the approach distance of the tip from a reference height (z_{ref}) is adjusted to the topography by either the recorded response ($Δf_{trigger}$) or the height limit (z_{limit}). **b** Example of experimental *Δf(z)* curve with fit of empirical model. **c** Map of elasticity values determined from 3D-AFM data with fits of empirical model to each 1D *Δf(z)* curve.