May Chemical Design of Molecular Vibrations Provide Means to Rationally Control Dynamics & Function of Single-Molecules?

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Understanding the motion/dynamics of a single molecule over a surface is a problem of a paramount importance in designing advanced molecular nanostructures/assemblies capable of meeting specific needs[1,2,3]. The interest is better realized by the broad spectrum of promising applications including molecular electronic devices, tribology/corrosion inhibition, and 3D nanopatterning[4]. One possible route to achieve a higher control on molecular diffusion along predetermined pathways would be to access the single-molecule mechanics during their on-surface displacements[5]. This in turn would provide a mean to rationally design molecules with improved assembly/diffusion properties. Nevertheless, to date, understanding the interplay between molecule mechanics, surface displacements and dynamics at a atomic level is highly challenging as it requires knowing not only the forces needed to manipulate them but also to relate them with particular molecular/atomic motion.

Almost 20 years passed after the first scanning probe microscopy[6] atomic-manipulation until it became possible to record the time variations of mechanical forces during manipulation[7]. As this technique[7,8,11,12,13,14] – *cryo-force-spectroscopy* – relies on a dynamic AFM operated at 4.8K in Ultra-High-Vacuum it allow us to perform successive manipulations a in a clean and controlled environment but also enable us to characterize both the surface and the molecule with atomic resolution prior and after the manipulation. This breakthrough opened new and exciting possibilities to explore mechanical properties at a single molecule level with an unrepresented resolution and control over the system. In this talk I shall discuss some of the major achievement and the versatility of this technique including: the discovery of a state of almost vanishing friction of graphene nanoribbons when sliding over a gold surface[8,9,10]; measuring the stiffness of a single DNA nucleotide and the detection[11] of a C-C bond twist at a single bond level[12]. Altogether this provides a comprehensive understanding of complex on-surface dynamics of the molecules over surfaces and how dynamic balancing of intra-molecular mechanics and surface comensurability play out in a broad range of conditions. At last, and with the aim of generalizing the importance of a chemical design of molecular vibrations, we show how DNA activity can be regulated through a physical code hidden in its sequence[15,16].

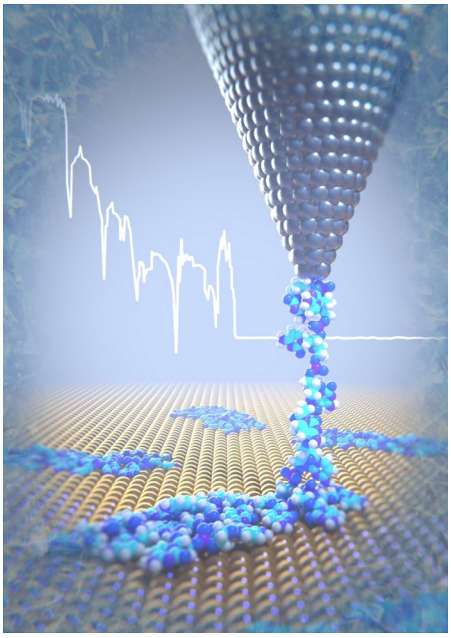

Figure 1*: Single molecule cryo-force spectroscopy: Lifting a single-stranded DNA molecule deposited over Au(111).*

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