Directional Motion of Single Molecules on Surfaces

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Molecular motion at surfaces is central to a wide range of processes, including the growth of two-dimensional materials, heterogeneous catalysis, and on-surface polymerisation. In thermally equilibrated systems, such motion is inherently random, as dictated by the principle of microscopic reversibility [1]. Nevertheless, gaining control over the motion of individual molecules is highly desirable, as it could enable the fabrication of novel materials or the development of more efficient catalytic systems.

I will first demonstrate how local gradients within the tunnel junction of a scanning tunnelling microscope can induce directed, unidirectional motion. In particular, an inhomogeneous electric field can be exploited to manipulate a single molecule through its internal dipole moment. The resulting motion consists of rotation about a fixed pivot point, which arises from the interaction between an oxygen atom in the molecule and a silver atom of the underlying surface [2]. When this anchoring interaction is disrupted, the motion evolves into a combination of rotational and translational components [3,4], which can be tuned through the choice of manipulation parameters.

Even more intriguing are molecular motors that exhibit intrinsic directionality—systems capable of converting external energy into motion along a predefined direction. An example of such a system which will be presented is based on the well-known Feringa motor. In these molecules, unidirectional rotation about a C-C double bond is achieved by sequential steps of photoisomerization and helix inversion. However, such motors frequently suffer from reduced performance or complete loss of function when transferred from solution to a metallic surface. In the final part of this talk, I will present a new molecular motor concept that overcomes this limitation. Using a small and structurally simple molecule, perfect unidirectionality is achieved upon adsorption on a Cu(110) surface [5]. The motion is driven by switching between two potential energy landscapes, thereby circumventing microscopic reversibility and yielding 100% unidirectional motion. Moreover, this controlled motion can be harnessed to perform work, such as transporting small cargo molecules across the surface.

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[2] G. J. Simpson et al, Nat. Commun., 10, 4631 (2019)
[3] G. J. Simpson et al, J. Phys. Chem. Lett. 14, 2487 (2023)
[4] B Ramsauer et al, J Phys. Chem. A, 127, 2041 (2023)
[5] G. J. Simpson et al, Nature, 621, 82-86 (2023)