

SINGLE-MOLECULE REACTIONS - IMAGING CHEMICAL BONDS AND TUNING ELECTRONIC STRUCTURE

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Abstract

Organic molecules provide a versatile, abundant, and cost-effective platform for the development of functional materials in many technologically relevant fields, such as electronics and photovoltaics. Effective utilization of molecular systems relies on control of structure, arrangement and bonding between molecular units, as well as an understanding on how these parameters affect the physical and chemical properties of the material.

Our studies focus on atomic-level investigations of surface-supported intra- and intermolecular reactions of organic molecules along with changes of their electronic properties. In particular, we resolved the bond rearrangements associated with cyclization reactions of single enediyne molecules by imaging the precise chemical structure of reactants and products (Fig. 1a), as well as intermediate species, using non-contact atomic force microscopy (nc-AFM). We used scanning tunneling microscopy and spectroscopy (STM/STS) to study the formation of low-energy extended electronic states in conjugated polymer chains, which were synthesized by radical polymerization reactions on metal surfaces (Fig. 1b). Additionally, we show how backgated graphene devices can be used to change the alignment of the electronic levels of organic molecules thus opening up the possibility to control their chemical and physical properties.

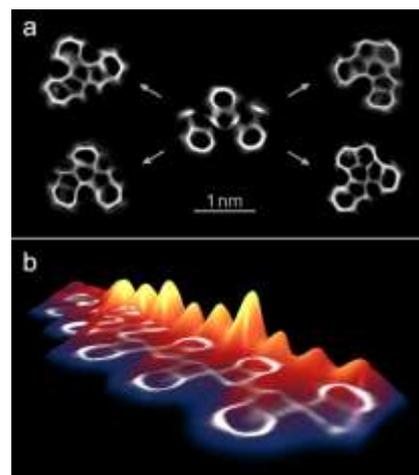


Fig. 1 (a) Nc-AFM measurements showing the chemical structures of reactants and products of competitive pathways of an enediyne cyclization reaction on Ag(100). (b) Three-dimensional representation of a simultaneous nc-AFM and STM measurement of an individual conjugated polymer chain on Au(111). The nc-AFM measurement reflects the chemical structure of the 4-nm-long polymer (shown in white). In contrast, the STM measurement is sensitive to the electronic local density of states of the polymer's lowest unoccupied molecular orbital (shown in blue-red-yellow).

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