Self-assembly and on-surface Decyanation of Tetracene Derivatives on Coinage Metal Surfaces

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We will present a study on the self-assembly and subsequent surface-assisted decyanation upon thermal activation of cyano-functionalized tetracene derivatives on coinage metal surfaces, also focusing on the role of the catalytic activity of the substrate. Two different tetracene derivatives were used: tetracyano-dihydrotetracene (4CN) and dicyano-diaryltetracene (2CN)[1]. Deposition of the molecules onto the single crystal substrates was carried out at room temperature under ultrahigh vacuum (UHV) conditions and different structures were obtained depending on the substrate. On Au(111) the molecules preferably assembled in a closed-packed structure, while on Cu(111) the formation of linear chains was preferred. On both substrates decyanation upon thermal annealing was observed. The reaction products and pathways were characterized by a combination of low-temperature high-resolution scanning tunneling microscopy and density functional theory calculations. Our findings present a new possibility for on-surface reactions of carbon-based nanostructures based on surface-assisted decyanation reactions.

1. N. Kerisit, P. Gawel, B. Levandowski, Y.-F. Yang, V. Garcia-Lopez, N. Trapp, L. Ruhlmann, C. Boudon, K. N. Houk, and F. Diederich, Chemistry – A European Journal (2018), 24, 159-168