

Abstract Submitted
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Molecular lifting, twisting, and curling during metal-assisted polycyclic hydrocarbon dehydrogenation. DAVIDE CURCIO, LUCA OMI-CIUOLO, Univ of Trieste - Trieste, Italy, MONICA POZZO, London Centre for Nanotechnology, University College London, UK, PAOLO LACOVIG, SILVANO LIZZIT, Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy, NAILA JABEEN, Univ of Trieste - Trieste, Italy, LUCA PETACCIA, Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy, DARIO ALFE, London Centre for Nanotechnology, University College London, UK, ALESSANDRO BARALDI, Univ of Trieste - Trieste, Italy — Through a combined experimental and theoretical approach, we show that coronene molecules adsorbed on Ir(111) undergo major changes in conformation during the dissociation process, which brings the molecules from a flat configuration to graphene, through a series of exotic configurations. The complex reaction path involves the tilting upwards of the molecules, which subsequently experience a rotation with respect to the surface. During the lifting, the C-C strain is initially relieved, while as the dehydrogenation proceeds, the molecules experience a progressive increase in the average interatomic distance, and gradually settle to form peculiar dome shaped nanographenes. This reaction mechanism can provide new insight into the surface assisted break-up mechanism of PAHs, which has been demonstrated to be an effective strategy for the synthesis of low dimensional carbon-based materials. Beside the peculiarity of the reaction pathway, using these processes we envisage the unique possibility of creating new structures with different functionalities by encapsulating single atoms below the carbon dome.

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