Electronic band structure of ultrathin on-surface synthesized zigzag chains

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On-surface synthesized Graphene nanoribbons (GNRs) [1] and oligophenylene chains [2] provide a vast playground for developing organic semiconductors with distinct electronic properties. Studies on aligned poly-(paraphenylene) and armchair-GNRs resulted in highly dispersive electronic bands with large HOMO-LUMO gap [3,4]. However, generating non-straight atomically precise and per fectly aligned chains allows us to go beyond the use of local techniques (STS) and complement it with averaging techniques (ARPES). Combining on-surface synthesis processes and the use of vicinal Ag(111) surfaces we achieved the formation of a monolayer of poly-(metaphenylene) (PMP) zigzag chains for the first time. We use STS and ARPES techniques to unraveled the band structure and HOMO-LUMO gap of zigzag chains. We find that the electronic structure presents weakly dispersive bands with an increase of its gap that is compatible with 1D electron confinement within straight sections. Both magnitudes are observed to vary with the straight section length following a 1/N tendency. These results, supported with DFT calculations, suggest a strong tunability of the polymer's electronic properties that can be correlated to its topology [5].

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