Revealing the electronic structure of a hybrid graphene-biphenylene nanoribbon family

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The application of graphene derivatives in semiconductor devices requires band gap tuning, which can be achieved by chemical doping, with the insertion of nanopores and non-hexagonal rings in 2D layers or the design of nanoribbons.

The bottom-up on-surface synthesis approach in ultra-high vacuum, allows for the fabrication of, e.g., atomically well-defined graphene nanoribbons (GNRs) or biphenylene nanoribbons (BPRs). Merino *et al.*[1] presented low-temperature scanning tunneling microscopy/spectroscopy (LT-STM/STS) data interpreted in terms of armchair-GNRs (AGNRs) with varying width obtained via lateral fusion of hydrogenated poly-para-phenylene chains (3-AGNRs) on Au(111). A systematic reduction of the band gap and a Fermi level pinning with increasing width was reported. Fan *et al.*[2] recently showed with LT-STM/STS and non-contact atomic force microscopy (NC-AFM) that width-varying BPRs can be achieved via the fusion of hydrofluorinated 3-AGNRs on Au(111), featuring a semiconducting to metallic and a direct to indirect band gap transition.

However, the combination of graphene and biphenylene segments into a single nanoribbon remains a challenge. Here, inspired by recent findings,[3] we revisit the fusion of hydrogenated 3-AGNRs on Au(111) using NC-AFM. Beyond the previously reported (3*p*)-AGNRs, we identify hybrid nanoribbons comprising graphene and biphenylene segments (see Figure 1). We thus introduce a new nano-architecture combining 3-GNRs, 6-AGNRs and biphenylene segments in a periodic fashion. LT-STS and density functional theory calculations show a reduction along with a transition from direct to indirect band gap as the ribbons become wider. This family of hybrid BP-GNR represents novel all-carbon scaffolds never reported so far.

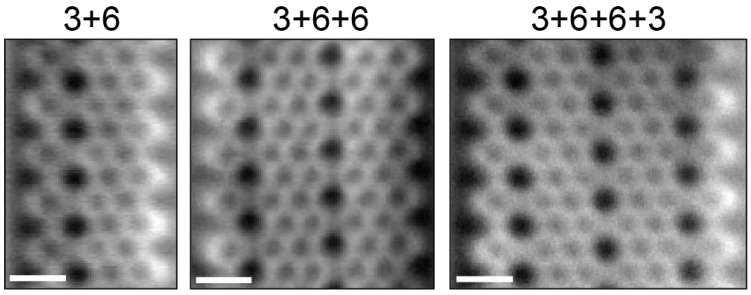

Figure 1. Three examples of the hybrid BP-GNR family.

References:

[1] N. Merino-Díez, et al. ACS Nano **11**, 11661 (2017).

[2] Q. Fan, et al. Science **372**, 852 (2021).

[3] P. Angulo-Portugal, et al. Submitted (2025).