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Electronic and Optical Properties of Atomically Precise Graphene Nanoribbons and Heterojunctions

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Among graphene related materials, nanoribbons (GNRs) – narrow stripes of graphene – have emerged as promising building blocks for nanoelectronic devices. The lateral confinement in GNRs opens a bandgap that sensitively depends on the ribbon width, allowing in principle for the design of GNR-based structures with tunable properties. However, structuring with atomic precision is required to avoid detrimental effects induced by edge defects. Recently, we have introduced a versatile route for the bottom-up fabrication of GNRs [1], allowing for the atomically precise synthesis of ribbons with different shapes as well as heterojunctions be-tween doped and undoped ribbon segments [2,3]. Here, we report on detailed experimental and computational investigations of the structural, electronic and optical properties of selected GNRs and heterojunctions [1-3]. For the case of armchair GNRs of width N=7, the electronic band gap and band dispersion have been determined with high precision [4,5]. Optical characterization has revealed important excitonic effects [6], which are in good agreement with ab initio calculations including many-body effects. For the case of heterojunctions, consisting of seamlessly assembled segments of pristine (undoped) graphene nanoribbons and deterministically nitrogen-doped graphene nanoribbons, we find a behavior similar to traditional p–n junctions. With a band shift of 0.5 eV and an electric field of 2 $\times$ 108 V m–1 at the heterojunction, these materials bear a high potential for applications in photovoltaics and electronics. Finally, we will discuss the potential of the bottom-up approach with regard to the fabrication of GNRs exhibiting zigzag edges, which are predicted to exhibit spin-polarized edge states.

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