Atomically precise graphene nanoribbon heterojunctions

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Graphene nanoribbons (GNRs) are one-dimensional strips of graphene that exhibit novel electronic and magnetic properties. Due to quantum confinement, GNRs exhibit a finite band gap and hold promise for future nano device applications. Here we report the bottom-up fabrication of GNR heterojunctions using a single molecular precursor, which allows atomically precise structural control of GNRs, thus enabling tuning of properties such as bandgap and heteroatom doping. The GNRs incorporate sacrificial carbonyl groups along their edges, and are formed through surface-assisted polymerization of molecular precursors via thermal annealing. Further annealing induces dissociation of GNR edge functional groups and leads to the formation of atomically precise type II heterojunctions between carbonyl functionalized segments and non-functionalized segments. The chemical structure of these GNR heterojuctions is revealed by bond-resolved scanning tunneling microscopy and non-contact atomic force microscopy. Scanning tunneling spectroscopy shows that GNR segments on either side of the atomically precise heterojunction interfaces exhibit a band alignment consistent with type II heterojunction behavior. Experimental band edge energy level alignment and wave function distributions agree well with *ab initio* theoretical simulations for this heterojunction system.