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Band alignment in atomically precise graphene nanoribbon junctions CHUANXU MA, LIANGBO LIANG, KUNLUN HONG, AN-PING LI, Oak Ridge National Laboratory, ZHONGCAN XIAO, WENCHANG LU, JERRY BERNHOLC, North Carolina State University — Building atomically precise graphene nanoribbon (GNR) heterojunctions down to molecular level opens a new realm to functional graphene-based devices. By employing a surface-assisted self-assembly process, we have synthesized heterojunctions of armchair GNRs (aGNR) with widths of seven, fourteen and twenty-one carbon atoms, denoted 7, 14 and 21-aGNR respectively. A combined study with scanning tunneling microscopy (STM) and density functional theory (DFT) allows the visualization of electronic band structures and energy level alignments at the heterojunctions with varying widths. A wide bandgap (˜2.6 eV) has been identified on semiconducting 7-aGNR, while the 14-aGNR appears nearly metallic and the 21-aGNR possesses a narrow bandgap. The spatially modulations of the energy bands are strongly confined at the heterojunctions within a width of about 2 nm. Clear band bending of about 0.4 eV and 0.1 eV are observed at the 7–14 and 14–21 aGNR heterojunctions, respectively. This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

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