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Graphene nanoribbons (GNRs) – one-dimensional strips of graphene – produced by bottom-up synthesis are considered promising candidates for next-generation integrated circuits of nanoscale dimensions. Careful design of the precursor molecules gives unprecedented atom-scale control over the GNR structure, electronic properties and also allows the formation of GNR junctions. However, theoretical understanding of overarching structure-property relationships in such systems is still eluding. Using tight-binding models, density functional theory and Green's function method [1], we determine the electronic properties of both experimentally synthesized and theoretically proposed GNR nanostructures containing quantum-dots [2], integrated metal-semiconductor-metal junctions [3] as well as experimentally observed defects [4,5]. Moreover, we address the electronic transport properties of angled two-terminal GNR junctions, which are inevitable as the interconnects in potential nanocircuits by high-throughput screening of hundreds of thousands of distinct configurations. We reveal the roles played by the bipartite symmetry of graphene, localized resonant states and geometry of the junction on the electronic transport properties. Overall, our work defines the guidelines for engineering GNR junctions with desired electrical properties and proposes novel device components, such as switches, splitters and transistors.

References

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Figures

