Graphene Nanoribbon Junctions as Elementary Components of Nanoelectronic Circuits

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On-surface chemical self-assembly of graphene nanoribbons (GNRs) has opened the possibilities for producing complex graphene-based nanostructures with atomic precision [1]. Two- and multiterminal junctions of GNRs synthesized using this bottom-up approach can be considered as elementary components of complex all-graphene nanoelectronic circuits [2]. We aim at establishing the design principles of such graphene-based nanoelectronic circuits by revealing the relations between the structure of GNRs junction and their electronic transport properties. The work is performed by means of first-principles and model Hamiltonian calculations combined with exhaustive high-throughput screening. We first focus on two-terminal GNR junctions with linear configurations being the simplest examples for which a sufficient body of experimental results is available (e.g. Refs. 3-6). Angled GNR junctions are more complex and are inevitable in the interconnects of nanoelectronic circuits. We systematically address the electronic transport properties of 60 and 120 degrees angled GNR junctions exploring ca. 400,000 distinct configurations, which allows us to formulate general guidelines into the engineering of transport properties of GNR circuits and identify a large number of junctions that have conductance close to the limit defined by the ballistic conductance of ideal GNR leads [7]. A user-friendly online application for modeling and calculation of the electronic transport properties of GNR junctions is presented [8]. Finally, I will discuss perspectives of designing transistors based on three-terminal GNR junctions [9].

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