Half-semimetallicity in graphene nanoribbon/hexagonal boron nitride heterojunctions

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Half-metals have been envisioned as active components in spintronic devices by virtue of their completely spin-polarized electrical currents. Actual materials hosting half-metallic phases, however, remain scarce. Using first-principles calculations, we predict that recently fabricated heterojunctions of zigzag nanoribbons embedded in two-dimensional hexagonal boron nitride are half-semimetallic, featuring fully spin-polarized Dirac points at the Fermi level. The half-semimetallicity originates from the transfer of charges from hexagonal boron nitride to the embedded graphene nanoribbon. These charges give rise to opposite energy shifts of the states residing at the two edges, while preserving their intrinsic antiferromagnetic exchange coupling. We further propose a simple mean-field Hubbard model Hamiltonian to capture the essential physics. Our findings demonstrate that these heterojunctions realize tunable one-dimensional conducting channels of spin-polarized Dirac fermions seamlessly integrated into a two-dimensional insulator, thus holding promise for the development of carbon-based spintronics.

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