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Thermal spin filtering effect and giant magnetoresistance of half-metallic
graphene nanoribbon co-doped with non-metallic Nitrogen and Boron

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ABSTRACT

Ab initio calculations based on density functional theory and non-equilibrium Green's function are performed to investigate the thermal spin transport properties of single-hydrogen-saturated zigzag graphene nanoribbon co-doped with non-metallic Nitrogen and Boron in parallel and anti-parallel spin configurations. The results show that the doped graphene nanoribbon is a full half-metal. The two-probe system based on the doped graphene nanoribbon exhibits various excellent spin transport properties, including the spin-filtering effect, the spin Seebeck effect, the single-spin negative differential thermal resistance effect and the sign-reversible giant magnetoresistance feature. Excellently, the spin-filtering efficiency can reach nearly 100% in the parallel configuration and the magnetoresistance ratio can be up to $-1.5 \times 10^{10}\%$ by modulating the electrode temperature and temperature gradient. Our findings indicate that the metal-free doped graphene nanoribbon would be a promising candidate for spin caloritronic applications.

Keywords: graphene nanoribbon; first-principles; half-metal; thermal spin transport; magnetoresistance

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