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Giant Electromechanical Response in Graphene Nanoribbons

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— The demonstration of spin injection into graphene has proposed that graphene could play a role in spintronic devices. Specifically, it has been found that zigzag graphene nanoribbons (ZGNR) have spin states at their edges. In this study, first principles quantum mechanical calculations have been performed to investigate the effect of twist on the electronic, magnetic and transport properties of ZGNR. We investigate the electronic and magnetic structures of nanoribbon of ZGNR in the flat geometry and with 180^0 twisting. Using density functional theory coupled with nonequilibrium Green's function method implemented in SIESTA code, we examine the local magnetic moments and the quantum conductance of twisted ZGNR in its ground state (antiferromagnetic) and in case of ferromagnetic spin orientations. Our calculations show that ZGNR in its ground state is insensitive to twisted deformation, since the conductance of the twisted ZGNR is almost unchanged, as well as, no band gap change. However, we observe electromechanical switch via twisting a ferromagnetic ZGNR in hypothetical ferromagnetic nanoribbons. The transmission in a hypothetical ferromagnetic state for 4-ZGNR is 2 quantum of conductance, while the transmission becomes zero in case of oppositely polarized leads (after twisting), i.e. we observe an ideal spin valve. We relaxed both the atomic positions and the spin directions in our calculations allowing for a Bloch/Neel-like domain wall in the latter case.

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