Giant Electromechanical Response in Graphene Nanoribbons
NABIL AL-AQTASH, RENAT SABIRIANOV, University of Nebraska at Omaha,
HONG LI, Peking University, Beijing, P.R. China, LU WANG, WAI-NING MEI,
University of Nebraska at Omaha, JING LU, Peking University, Beijing, P.R. China
— 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° 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 deforma-
tion, 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 fer-
romagnetic 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.

Nabil Al-Aqtash
University of Nebraska at Omaha

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