Magnetoelectric and Flexomagnetic effects in hybrid C/BN nanostructures

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It has been predicted that, under a corrugating distortion, two-dimensional non-centrosymmetric crystals become strongly polarized in the plane of the film, with a nonlinear electromechanical effect. Hence, polar hexagonal BN monoatomic sheets are expected to exhibit not only piezoelectricity but also an unusual flexoelectricity [1]. Surprisingly, similar corrugations would induce a gap opening in graphene [2]. The realization of hybrid C/BN monoatomic sheets [3] with potential half-metallic properties [4], opens the possibility to achieve multifunctional properties in a graphene-like structure, where electro-magneto-mechanical properties can be tuned externally by application of an external perturbation (electric or magnetic fields, mechanical strains, etc). In this contribution we will present first-principles density functional calculations to show strong magnetoelectric (ME) effects in hybrid nanostructures made from C and BN domains with zigzag interfaces. This effect originates from the magnetic properties of graphene's zigzag edges and the dielectric properties of the latter, and is highly anisotropic because of the different properties of the C-B and C-N bonds. For nanotube geometries, the linear ME coefficient compares to that of prototypical Cr2O3, whereas for 2D monolayers, the surface ME coefficient is larger than the one predicted for graphene nanoribbons on silicon substrates. Band shifts and gap modulations (also seen in pure BN and C nanotubes) are observed and can give rise to an inversion of the spin of half-metallic states, which would allow for electric-field control of conducting spins at graphene nanoconstrictions embedded in BN sheets. Flexomagnetic effects will also be discussed for corrugated planes made out of BN and C strips with zigzag edges.

References

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