Mechanical-Electric-Magnetic Coupling Effects in Functional Nanomaterials

Wanlin Guo [a] Zhuhua Zhang

State Key Laboratory of Mechanics and Control of Mechanical Structures and MOE Key Laboratory for Intelligent Nano Materials and Devices, Institute of Nanoscience, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, China

At nanoscale, matters show distinctly different behaviors from their bulk materials mainly due to the strong coupling between the local fields of matter consisting of electronic structures, charge, orbital and spin states and external applied fields. Such nanoscale multifield couplings can turn very common materials such as carbon, even insulating boron nitride, into functional nanomaterials with fantastic properties we expected for nanoelectronics, spintronics as well as energy conversion devices.

We predict a magnetoelectric (ME) effect in graphene nanoribbons on silicon substrates by first-principles calculations [1]. It is shown that a bias voltage can produce strong linear ME effect by driving charge transfer between the nanoribbons and substrate, as shown in Figure 1, thus tuning the exchange splitting of magnetic edge states; moreover, the bias induced n-to-p-type transition in the ribbon layer can switch the ME coefficient from negative to positive due to the unique symmetry of band structures. This mechanism is proven to be robust against variations in material and physical configurations, thus opening a new avenue for ME coupling in metal-free magnet systems of practical importance. We have also systematically studied bias-voltage-induced modulation of magnetic and electronic properties of bilayer zigzag graphene nanoribbons (Z-GNRs) on Si(001) substrate by first-principles calculations [2]. We show that the intrinsically nonmagnetic bilayer Z-GNRs exhibit magnetic ordering on the top layer while the bottom layer serves as a nonmagnetic buffer layer when adsorbed on the substrate.Interestingly, the adsorbed bilayers display distinct ribbon-width-dependent magnetoelectric effect under bias voltages. The magnetoelectric coefficient oscillates with increasing ribbon width, which arises from an interesting interplay of the interaction of the bottom ribbon layer with the substrates and the decay length of the localized edge states in Z-GNRs. We demonstrate from density-functional theory calculations that strong spin polarization can be achieved on a silicon surface via chemisorption of graphene nanoribbons (GNRs) [3]. The net electron spins are due to the unique silicon dangling-bond states induced by the chemisorption of GNRs and further localized by the well-aligned Si-C bonds between the silicon surface and the GNRs. The induced magnetic moment on the silicon surface depends on the width of GNRs and is thus tunable through controlling lateral separation among GNRs. We show that the silicon surface magnetization can even sustain large vertical compression to the GNRs and thus can be used as a functional switch upon high deformation of GNR.

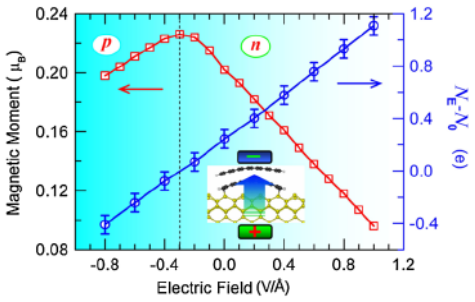
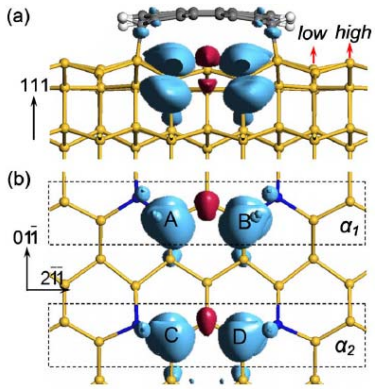


Figure 1. Charge transfer induced ME effect in the adsorbed bilayer Z7-GNR on Si(001) substrate. Blue line with circles: The amount of charge transferred to the top GNR layer as a function of electric field strength. NE and N0 present the total number of electrons in the top GNR layer under bias voltage and those in a neutral freestanding Z7-GNR, respectively. Red line with squares: magnetic moment per edge carbon atom of A sublattice in the top layer as a function of the field strength. [1]



[a] Corresponding author. Email: wlguo@nuaa.edu.cn

Figure 2. The most stable geometric configuration for a Z_4-GNR adsorbed on Si(111) and computed magnetic density distribution. [(a) and (b)] Side and top views of the magnetization density (0.005 e/Å^3), respectively. The Z_4-GNR is removed in (b) for clarity, and all the silicon atoms bonding to the GNR are distinguished in blue (dark). Magnetization densities in two spin directions are distinguished by light blue (light grey) and magenta (dark grey), respectively. [3]

We have studied the electronic and magnetic properties of zigzag graphene nanoribbons with protruded steps along their edges (ZS-GNRs) by extensive density-functional theory calculations [4]. The electronic and magnetic properties are determined by an interesting interplay between the length of the protruded step and the distance of two adjacent steps along the ribbon edge. With a small length of the protruded steps along the edge, the system can be converted from a nonmagnetic semiconductor to metal and then to a magnetic semiconductor by increasing the step-to-step distance. In particular, the energy gap decreases first toward a zero minimum and then gradually increases as the step length increases, accompanying with the rapid increase in the edge magnetization. When the step length exceeds a critical value, the ZS-GNR will be always a magnetic semiconductor regardless of the step-to-step distance. We examine the magnetic properties of two-dimensional graphene with topological line defect using first-principles calculations and predict a weak ferromagnetic ground state with spin-polarized electrons localized along the extended line defect [5]. Our results show that tensile strain along the zigzag direction can greatly enhance local magnetic moments and ferromagnetic stability of the system. In sharp contrast, tensile strain applied along the armchair direction quickly diminishes these magnetic moments. A detailed analysis reveals that this intriguing magnetism modulation by strain stems from the redistribution of spin-polarized electrons induced by local lattice distortion. It suggests a sensitive and effective way to control magnetic properties of graphene which is critical for its applications in nanoscale devices. Moreover, strain tunable magnetism has also been found in carbon doped silicon nanowires.

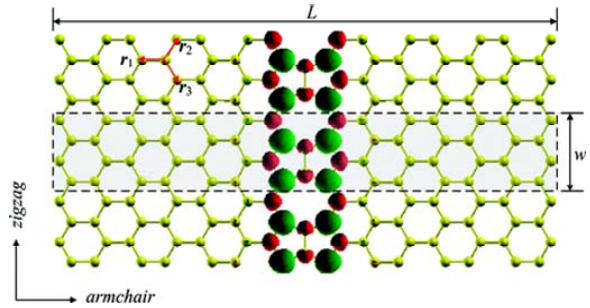


Figure 3. The computed magnetic density distribution of a graphene sheet with line defect. [5]

Those extraordinary mechanical-electric-magnetic coupling effects in graphene systems open up new vistas in functional devices compatible with silicon-based technology and nanotechnology for efficient energy conversion, self-powering flexible devices and novel functional systems.

References

[1] Zhang Z., Cheng C., Guo W.: Magnetoelectric Effect in Graphene Nanoribbons on Substrates via Electric Bias Control of Exchange Splitting. *Phys. Rev. Lett.* **103**: 187204, 2009.

[2] Zhang Z., Cheng C., Zeng X., Guo W.: Tuning the magnetic and electronic properties of bilayer graphene nanoribbons on Si(001) by bias voltage. *Phys. Rev. B* **81**: 155428, 2010.

[3] Zhang Z., Guo W., Zeng X.: Tunable magnetism on Si(111)-(2×1) via chemisorption of graphene nanoribbons. *Phys. Rev. B* **82**: 235423, 2010.

[4] Wu W., Zhang Z., Lu P., Guo W.: Electronic and magnetic properties of zigzag graphene nanoribbons with periodic protruded edges. *Phys. Rev. B* **82**: 085425, 2010.

[5] Kou L., TangC., Guo W., Chen C.: Tunable Magnetism in Strained Graphene with Topological Line Defect. *ACS Nano* **5**: 1012–1017, 2011.