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Unveiling multiferroic proximity effect in graphene

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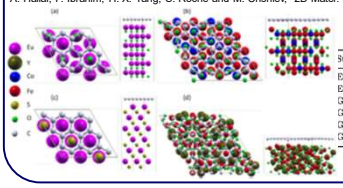
ABSTRACT

Graphene in proximity of magnetic material has been attracting a lot of interest in view of possible spintronic application in vertical and lateral junctions [1-3]. Multiferroics, co-exhibiting a magnetic (M) and ferroelectric (P) order, constitute an interesting class of magnetic insulators that bring about an additional parameter in play that is the electric polarization P. Using first-principles calculations, we report the multiferroic-induced proximity effect (MFPE) in graphene proposing the concept of controlling its electronic and magnetic properties via multiferroic substrate. We consider bismuth ferrite $BiFeO_3$ (BFO) whose room-temperature multiferroicity promotes it as a good candidate for applications [4]. We show that the spin-dependent electronic structure of graphene is strongly impacted both by M and P in the underlying BFO. Based on extracted Hamiltonian parameters obtained from the graphene band structure, we propose a concept of six-resistance device based on exploring multiferroic proximity effect giving rise to significant proximity electro- (PER), magneto-(PMR), and multiferroic (PMER) resistance effects [5]. This finding paves a way towards multiferroic control of magnetic properties in two dimensional materials.

Introduction

Tailoring magnetic insulator proximity effect in graphene

A. Hallal, F. Ibrahim, H. X. Yang, S. Roche and M. Chshiev, 2D Mater. 4, 025074 (2017)

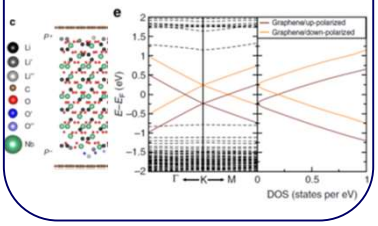


Structure	E_G (meV)	$\Delta_\uparrow$ (meV)	$\Delta_\downarrow$ (meV)	δ_c (meV)	δ_h (meV)	E_D (eV)
EuO/Gr/EuO(1BL) aligned[53]	127	309	344	182	217	-2.8
EuO/Gr/EuO(1BL) misaligned[53]	-38	137	182	211	220	-2.8
GR/EuO(6BL)	50	134	98	84	48	-1.37
GR/EuS(6BL)	160	192	160	23	-10	-1.3
Gr/$Y_3Fe_5O_{12}$	1	116	52	-52	-115	-0.78
Gr/$CoFe_2O_4$	-37	12	8	-45	-49	+0.49

[55] S. Su, Y. Barlas and R. K. Lake, arXiv:1509.06427 (2015)

Ferroelectrically driven spatial carrier density modulation in graphene

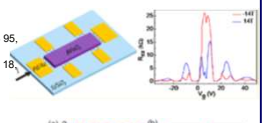
C. Baeumer, D. Saldana-Greco, J. M. P. Martirez, A. M. Rappe, M. Shim, and L. W. Martin, Nature Comm. 6, 6371 (2015)



Magnetic proximity effect in graphene coupled to $BiFeO_3$

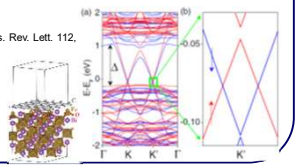
Experiment:

Y. F. Wu et al., Phys. Rev. B 95, 195426 (2017)
H-D. Song et al., Nano Lett. 18, 2435 (2018)



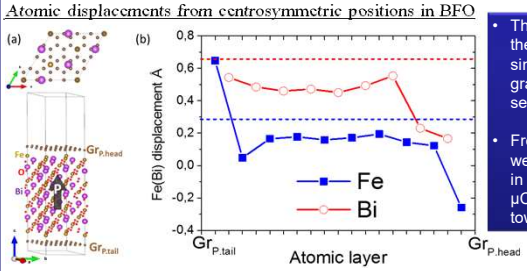
Theory:

Z. Qiao et al., Phys. Rev. Lett. 112, 116404 (2014)



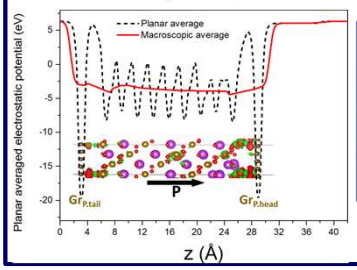
$Gr_{P.tail}$/BFO/$Gr_{P.head}$ heterostructure

Atomic displacements from centrosymmetric positions in BFO



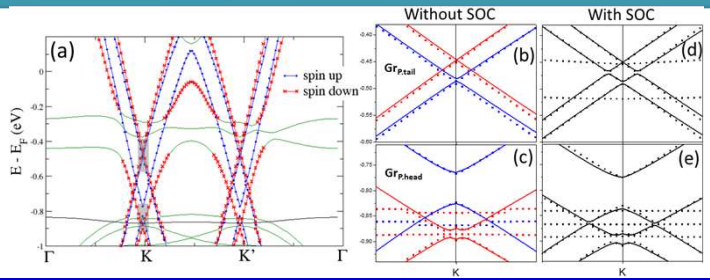
- The heterostructure provides the opportunity to compare simultaneously two different graphene layers relatively sensing opposite direction of **P**.
- From the atomic displacements we conclude that **P** is sustained in the BFO layers with P=63 μC/cm² and points from $Gr_{P.tail}$ towards $Gr_{P.head}$.

Planar & macroscopic averaged electrostatic potential



- Presence of **P** and polar surface charges lead to the formation of two different interfaces with graphene revealed by different adsorption distances.
- Stronger electrostatic interaction is observed at the *head* interface where the bound charges are quantitatively larger. This explains the larger induced spatial charges in the inset figure.

DFT band structure and fitted TB Hamiltonian



TB Hamiltonian describing the graphene's linear dispersion relation in proximity of a magnetic insulator

$$H = \sum_{i\sigma}\sum_{l} t_{l\sigma} c^{\dagger}_{(i+1)1\sigma} c_{i0\sigma} + h.c. + \sum_{i\sigma\sigma'}\sum_{\mu=0}^{1} [\delta + (-1)^{\mu}\Delta_{\delta}] c^{\dagger}_{i\mu\sigma} [\vec{m}\cdot\vec{\sigma}]_{\sigma\sigma'} c_{i\mu\sigma'} + \sum_{i\sigma}\sum_{\mu=0}^{1} [E_D + (-1)^{\mu}\Delta_s] c^{\dagger}_{i\mu\sigma} c_{i\mu\sigma}$$

Rashba spin-orbit coupling term

$$H_{soc} = it_R \sum_{i\sigma\sigma'}\sum_{l} c^{\dagger}_{(i+1)1\sigma} [\sigma^x_{\sigma\sigma'} d^x_l - \sigma^y_{\sigma\sigma'} d^y_l] c_{i0\sigma'} + h.c.$$

Spin-dependent energy band gaps, exchange splitting parameters, and parameters used to fit the TB Hamiltonian to the DFT band structure

	E_G(meV)	$\Delta_\uparrow$(meV)	$\Delta_\downarrow$	δ_c(meV)	δ_h	E_D(eV)	γ_{soc}(meV)	$t_\uparrow$(eV)	$t_\downarrow$	t_R(meV)
								2.66	2.3	
$Gr_{P.head}$	-48.6	55	26	104	75	-0.85	4	2.66	2.28	8.7
								2.61	2.32	
$Gr_{P.tail}$	-34	6	1.5	-35	-40	-0.47	5	2.42	2.5	7.5

Spin-dependent transport (scattering matrix formalism)

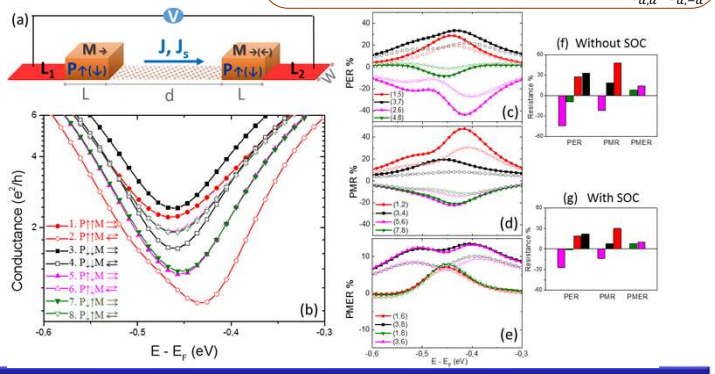
Conductance in the linear response regime

$$G^{\sigma,\sigma'}_{\alpha,\alpha'} = \frac{e}{h}\sum_{\sigma}\int T^{\sigma,\sigma'}_{\alpha,\alpha'}\left(\frac{-\partial f}{\partial E}\right) dE$$

Proximity electroresistance: $PER^{\sigma,\sigma'}_{\alpha,\alpha'} = \frac{G^{\sigma,\sigma'}_{\alpha,\alpha} - G^{\sigma,\sigma'}_{\alpha,-\alpha}}{G^{\sigma,\sigma'}_{\alpha,\alpha} + G^{\sigma,\sigma'}_{\alpha,-\alpha}}$

Proximity magnetoresistance: $PMR^{\sigma,\sigma'}_{\alpha,\alpha'} = \frac{G^{\sigma,\sigma}_{\alpha,\alpha'} - G^{\sigma,-\sigma}_{\alpha,\alpha'}}{G^{\sigma,\sigma}_{\alpha,\alpha'} + G^{\sigma,-\sigma}_{\alpha,\alpha'}}$

Proximity multiferroic resistance: $PMER^{\sigma,\sigma'}_{\alpha,\alpha'} = \frac{G^{\sigma,\sigma}_{\alpha,\alpha} - G^{\sigma,-\sigma}_{\alpha,-\alpha}}{G^{\sigma,\sigma}_{\alpha,\alpha} + G^{\sigma,-\sigma}_{\alpha,-\alpha}}$



- Model spintronic device used consists of two multiferroic regions on top of a graphene sheet.
- Conductance curves show six different resistance states two of which are degenerate.
- Different combinations of conductance states give rise to three types of proximity resistances.
- SOC doesn't change our results qualitatively but rather decreases the values of the conductances and consequently the values of the different types of proximity resistances.

Conclusions

- The magnetic proximity effect in graphene can be tuned by the electric polarization existing in the multiferroic substrate.
- Our findings: - propose additional degrees of control for proximity induced phenomena in graphene and perhaps in other two-dimensional materials.
  - lead to a concept of multi-resistance device based on the multiferroic proximity effect.

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5. F. Ibrahim et al., 2D Mater. 7, 015020 (2020)

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