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“Seamless” graphene interconnects for the prospect of all-carbon spin-polarized field-effect transistors

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Abstract

Magnetism in graphene nanofragments arises from the spin polarization of the edge-states; consequently, as the material inexorably shrinks, magnetism will become a dominant feature whereas the bulk carrier mobility will be less relevant. We have carried out an *ab initio* study of the role of graphene-ultra-nanofragment magnetism on electronic transport. We present, as a proof-of-concept, a *nanoscopic* spin-polarized field-effect transistor (FET) with the channel and metallic contacts carved from a single graphene sheet. We demonstrate the selective tuning of conductance through electric-field control of the magnetic, rather than the charge, degrees of freedom of the channel, the latter typically employed in *microscopic* graphene FETs.

Keywords

Spintronics; FET; graphene diamond; graphene ribbon

Similar to carbon nanotubes, graphene holds great promise for future electronics because of its outstanding electrical^{1,2}, mechanical³, and thermal⁴ properties. Because of its 2-dimensionality, however, graphene has the additional advantage for large-scale integration devices fabricated via solid-state lithographic techniques. The fabrication of all-carbon field-effect transistors (FETs), where the metallic leads, central dot, and gates are carved from a single sheet of graphite, is currently the subject of intense research^{5,6,7}.

Graphene displays exceptional high carrier mobility^{1,2} allowing for microscopic graphene FETs that are faster than their silicon counterparts⁸. On the other hand, as electronics taps into nano-scale graphene ribbons or fragments (< 50 nm), the edge states become dominant. These states are robust for any random-shaped graphene nanofragments as long as the underlying honeycomb lattice is not substantially modified⁹. The edge-states of graphene ultra-nanofragments have been predicted to be magnetic^{10,11}, where the various magnetic states lead to distinct electrical properties¹². This magnetic ordering may be the underlying origin of the experimentally observed conductance switching^{7,13} and band gap modulation^{14,15} in graphene nanofragments.

Following the silicon-electronics breakthrough microchip paradigm of (1) fabricating all necessary discrete electrical components and wiring from silicon and (2) integrating all these elements in the same silicon wafer, very-large-scale integration in all-carbon graphene devices will require (i) a robust building block analog to the silicon transistor, and (ii) seamless coupling of these nano-units through graphene nanoribbon interconnects, which will allow in turn for ballistic transport. Isolated diamond-shaped graphene flakes,

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henceforth referred as “diamonds”, are intriguing devices uniquely poised to evolve self-contained building blocks¹². They harness the magnetic and magneto-electro behavior predicted for graphene nanofragments to exhibit well defined magnetic states with distinct electrical conductance, which can be tuned through the electric field modulation of the local magnetism. The second requirement of graphene ribbon interconnects is even more important because it circumvents the use of foreign metallic (Al, Cu, Pd) contacts, which have overburden the microelectronics industry with undesirable interfacial problems. More critically, the charge doping induced by the mismatch in work function between the graphene and the foreign metallic contact extends over several hundreds of nanometers deep into the graphene layer^{16,17}, in contrast to the few atomic lengths in traditional semiconductor devices, thus degrading the performance and control of graphene FETs^{18,19}, especially as they approach nanometer sizes. The controlled fabrication, characterization, and identification of graphene nanofragments with well defined edges have been a challenge due to the experimental lack of high spatial resolution. However, state-of-the-art experiments on graphene have demonstrated growth and patterning of larger and higher quality films²⁰; controlled fabrication of sharp edges²¹⁻²³; and selective etching for structures with 120° and 60° angles^{24,25}.

The effect of edge-states of graphene nanofragments on the transport properties in all-carbon spintronics is of central interest and importance and it has not been addressed theoretically thus far. In this article we use *ab initio* electronic structure and Landauer-Büttiker transport calculations to demonstrate, as a proof-of-concept, that diamond graphene nanofragments can be *seamlessly* interconnected to carbon leads, acting as metallic contacts, while maintaining the diamond's key magneto-electric properties. Thus, these predictions suggest the possibility for carving ultra-dense all-carbon planar magnetic-based FETs from the same graphene single-layer wafer, as schematically shown in Figure 1.

The spin-polarized *ab initio* electronic structure calculations in the presence of constant electrostatic potential gradients were performed using the SIESTA method²⁶ with the generalized-gradient PBE exchange-correlation density functional²⁷. The valence electrons are expanded using localized basis of double- ζ -polarized character and Troullier-Martin pseudopotentials are used for the core electrons.

Isolated diamond graphene nanofragments

In Figure 2 we show the variation of the energy of the ferromagnetic (FM) and nonmagnetic (NM) configurations relative to that of the antiferromagnetic (AF) configuration for hydrogenated zigzag diamond-shaped graphene nanofragments as a function of the number N of phenyl rings along the horizontal diagonal of the diamond. The ground state is always AF with the spins of the upper and lower triangular subunits aligned antiparallel. The difference in total energy between the FM and AF configurations, ΔE_{FM} , is about 150 meV and independent of N . This is due to the fact that ΔE_{FM} is dominated by the exchange coupling between spins across the common edge of the upper and lower triangular subunits and mainly localized in the vicinity of the two horizontal vertices, which in turn do not scale with size. In sharp contrast, the energy of the NM configuration relative to the AF, ΔE_{NM} , increases linearly with N , since ΔE_{NM} involves the exchange coupling between all zigzag edge atoms in an edge. Thus, graphene diamond nanofragments are two-state (singlet-triplet) quantum systems robust against thermal fluctuations.

As a building block, it is equally important that the graphene diamond has a molecular band gap between the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO, respectively). An energy bandgap is a desirable feature for electronics because it determines the electrical and optical properties of the material. While bilayer graphene has

been found to exhibit a bandgap²⁸, this feature is notably absent in graphene, thus, limiting the versatility of microscopic single-layer graphene FETs. The HOMO-LUMO energy gap is plotted versus N in the inset in Figure 2; it decreases almost linearly with N , similar to graphene nanoribbons and vanishes at $N > 29$, corresponding to a diamond width of 7 nm. For $N = 22$ (diamond width of 5.4 nm) there is a still considerable bandgap of 0.2 eV.

A tunable band gap in the graphene-diamond building blocks is also highly desirable because it allows great flexibility in design and optimization of devices, in particular if it could be tuned by applying a variable external electric field. The fact that the energy gap in graphene diamonds is spin resolved is significant, since it provides an additional handle to electrically manipulate the spin current through the FET. In Figure 3a we show the electric field evolution of the frontier molecular orbital energies for the AF configuration of the $N = 8$ graphene diamond, where the electric field, F , is coplanar and applied along the larger diagonal of the diamond. We find that the zero-field spin-up HOMO-LUMO gap of 0.66 eV decreases to its minimum value of ~ 40 meV at ~ 0.23 V/Å. For $F > 0.23$ V/Å, the spin-up band gap increases until the diamond eventually undergoes a transition to its nonmagnetic state at ~ 0.73 V/Å. The field evolution of the spin-down HOMO-LUMO gap exhibits the opposite behavior. The progressive field-induced quenching of the spin magnetization as the graphene diamond undergoes the AF $\rightarrow$ NM transition is shown in Figure 3b.

Semi-Infinite graphene nanoribbon interconnects

In order to circumvent the aforementioned detrimental problems associated with foreign metallic interconnects and for the purpose of scalability, metallic wires fabricated from the same graphene wafer should be used to interconnect the graphene quantum dots. While zigzag nanoribbons have been predicted to be metallic²⁹, they present two main disadvantages in serving as interconnects. First, the zigzag edges are magnetic and hence would introduce more complexity into the transport properties of the FET^{30,31} and possibly affecting the magneto-electro properties of the graphene diamond. Second, the bandgap induced by the spin polarization³² reduces substantially the conductance of the interconnects.

There is increasing theoretical^{33,34} and experimental^{35,36} evidence suggesting that, in a hydrogen-deficient environment, the non-hydrogenated zigzag edge reconstructs into a more stable and self-passivated (5,7) edge comprised of alternating heptagons and pentagons along the ribbon. Moreover, the reconstruction of the edges eliminates the edge-states, and therefore magnetism, rendering the ribbons gapless. Thus, reconstructed nonmagnetic graphene nanoribbons can serve as metallic leads for interconnecting the graphene diamond into junctions. The all-carbon graphene-junction model (FET) employed in the electronic structure and transport calculations, shown in Figure 1c, combines both hydrogenated zigzag and non-hydrogenated (5,7)-reconstructed edges, and is intended as a proof-of-concept device. As a possible route for fabrication, we suggest, reconstruction of the edges by thermal annealing³⁷ and posterior direction-selective hydrogen plasma etching, with masking of the reconstructed areas³⁸, to taper the diamond's edges back to hydrogenated zigzag^{39,40}.

Magnetic graphene FET

The electronic transport through the graphene FET is calculated employing the combined density functional theory (DFT) and Green's function approach^{41,42}, in which the finite device scattering region M , shown in Figure 1c, is made infinite by mathematically attaching semi-infinite left and right (5,7)-reconstructed leads. The spin-dependent current, I^σ , in the graphene junctions is determined as a function of both the applied bias voltage V_{bias} and "gate" field F , from

$$I^\sigma(V_{bias}, F) = \frac{e}{h} \int_{-\infty}^{+\infty} dE \text{TF}^\sigma(E, F) \left[f(E - E_F - \frac{e \cdot V_{bias}}{2}) - f(E - E_F + \frac{e \cdot V_{bias}}{2}) \right], \quad (1)$$

where f is the Fermi function at 300 K, E_F is the Fermi level of the ribbon, and the spin-dependent transmission function, TF, at energy E and gate field F , is given by

$$\text{TF}^\sigma(E, F) = \text{Tr}[\Gamma_L G_M^\sigma \Gamma_R G_M^{\sigma\dagger}]. \quad (2)$$

Here, $\Gamma_{L(R)} = \sqrt{-1} \left(\sum_{L(R)} - \sum_{L(R)}^\dagger \right)$ is the coupling of the device region to the left (right) L (R) semi-infinite lead and the Green's function of the device region is

$$G_M^\sigma(E, F) = [ES_M - H_M^\sigma(F) - \sum_L - \sum_R]^{-1}, \quad (3)$$

where S_M is the overlap matrix. Our DFT calculations find that, both, the infinite (5,7)-reconstructed ribbon and the atoms within the device region which are neighbors to the leads are not magnetic (Figure 1c), in agreement with other calculations⁴³. Therefore the self-energies $\Sigma_{L(R)}$, involving the surface Green's function⁴¹ of the leads, are determined from non-spin-polarized DFT calculations of the infinite ribbon. Thus, the spin dependence enters solely through the Hamiltonian matrix H_M^σ of the device region.

The zero-bias and zero-gate-field total transmission function of the infinite (5,7)-reconstructed ribbon, shown in green in Figure 4a, shows multiple Bloch transmission channels evidenced by the integer stair-case shape, typical of crystalline nanowires, indicating a gapless metallic material. The introduction of a diamond graphene scattering center within the ribbon suppresses dramatically the electron transmission except at discrete transmission peaks corresponding to the frontier molecular orbitals of the isolated diamond (black curve in Figure 4a). This confirms that the transport in these FET junctions is dominated by the chemistry of the diamond, i.e. the transport is resonant (with TF = 1) through the molecular levels of the diamond, and not by the choice of metallic interconnecting leads. Consequently, the electrical properties of the FET could be controlled through gate-field tuning of the frontier energy levels of the diamond.

In Figure 4b we show the gate electric-field variation of the spin-up (blue) and spin-down (red) transmission function of the $N=8$ graphene diamond coupled to the (5,7)-reconstructed ribbon. The various thick blue curves denote the field-variation of the tips of the spin-up resonance peaks of the HOMO, HOMO-1, LUMO, and LUMO+1. The transmission amplitude of all peaks is unity, indicating ideal ballistic transport. At zero gate field the spin-up and -down MOs are degenerate, with an energy gap between the frontier transmission peaks of 0.49 eV, which is comparable to the HOMO-LUMO gap of 0.66 eV for the corresponding isolated diamond. Alike with the behavior of the isolated diamond, increasing the gate field causes the frontier spin-up (spin-down) transmission peaks to close (open) up around the Fermi level to a minimum (maximum) of 26 (580) meV at 0.25 (0.15) V/Å (Figure 4b), which in turn leads to an increase (decrease) in the spin-up (spin-down) current for a given V_{bias} voltage. For gate fields $F > 0.25$ V/Å, the spin-up transmission gap progressively reopens, and at $F \sim 0.6$ V/Å the system undergoes a transition into a nonmagnetic state. Note, that the spin-up HOMO/HOMO-1 and LUMO/LUMO+1

transmission peaks (thick blue curves) cross at ~ 0.40 V/Å, which is analogous to the band crossing at 0.38 V/Å for the isolated diamond (Figure 3a). This corroborates that the magnetoelectric properties exhibited by the graphene diamonds¹² are preserved in the presence of graphene ribbon interconnects.

The variation of the total current ($I = I^\uparrow + I^\downarrow$) with *gate* electric-field for various bias voltages is shown in Figure 5a. It demonstrates the modulation of the current with *gate* field F at a fixed bias, confirming the potential of this device not only as a magnetic *switch* but also as an *amplifier*, the two essential characteristics of a FET. The change of the dI/dF slope at $F \sim 0.15$ V/Å is due to a similar decrease of the energy-gap for the spin up channel, which is a consequence of the second-order Stark effect¹². This continuously tunable control of bandgap with electric field makes the graphene-diamond a promising optical modulator candidate, similar to the effect recently found in bilayer graphene^{44,45}, where the symmetry-breaking direction of the applied external field is not coplanar but perpendicular to both graphene sheets.

The electric-field tuning of the spin-resolved band gap of the diamond in the AF configuration (Figure 3a) gives rise to a spin-filtering effect, analogous to that predicted in graphene ribbons⁴⁶, which become half-metallic. In contrast to other proposed all-carbon spin filters that employ unreconstructed magnetic graphene ribbons^{47,48}, in this work, the current spin-polarization ratio, $CSP = (I^\uparrow - I^\downarrow)/(I^\uparrow + I^\downarrow) \times 100$, can be controlled via *gate* tuning of the spin-resolved band gap of the diamond. The CSP plotted as a function of *gate* field F in Figure 5b for various bias values shows that it can be manipulated from $\sim 95\%$ to 0% in the neighborhood of the AF→NM transition.

Although in this work we have considered diamonds with “perfect” hydrogenated zigzag edges, the underlying electric field mechanism lies on the relative spin alignment between the top and bottom triangular subunits of the diamond and not on transport through the edges *per se*. Moderate random geometrical distortions of the zigzag edges will not destroy the overall spin alignment^{46,49,50} and therefore, the device should be robust to deviations from perfect edges. Furthermore, the proposed concept may be extended to graphene nanofragments of random shapes and edges, since their magnetic ordering is also expected to be robust as long as the underlying honeycomb lattice is not substantially destroyed⁹.

It has been predicted that infinite zigzag-edge GNR can sustain spin-waves with relatively “short” spin-correlation lengths (~ 1 nm at 300 K)⁵¹. On the other hand, having a sub-10-nm-wide graphene diamond nanofragment as the central region, makes it less likely to sustain spin-wave excitations. Also, zigzag edges with angle turns of 120° and 60° act as domain walls that favor antiparallel and parallel coupling, respectively⁵¹, which should increase the correlation length in diamond-shaped nanofragments.

Although in principle FM ordering can only occur in infinitely large systems, the term FM or quasi-FM is often used for finite systems if the FM relaxation time (τ_{FM}) is large enough as in the case of the various proposed spintronic devices based on the FM ordering of zigzag graphene nanoribbons^{30,31}. Triangular nanofragments, which have been proposed as possible memory devices,⁵² have a finite but very large τ_{FM} , even for small size triangles. The relaxation time follows the Arrhenius-type scaling $\tau_{FM} \propto \exp [J_{eff} N^2 / 2k_B T]$, where $N+1$ is the number of phenyl rings along one edge. The N^2 dependence is a crucial consequence of the triangular shape and related to the fact that a spin interacts (J_{eff}) not only with its nearest neighbors (typical of nanomagnets) but with all the other spins in the triangle^{52,53}. Moreover, coupling to metallic carbon leads has been suggested to further enhance the FM ordering in the triangles⁵⁴. For the diamond graphene nanofragment in the AF configuration

one would expect a longer relaxation time because of the additional exchange coupling between the upper and lower triangular subunits.

This work is aimed as a proof-of-concept to stimulate the growing field of graphene spintronics, where rapid advances and discoveries in the study of graphene may meet, in the near future, the multiple technological challenges faced in the controlled fabrication and stabilization of all-carbon devices. For instance, alternative routes such as edge⁵⁵ and surface⁵⁶ doping can lead to edge-state enhancement and manipulation of the bandgap^{57,58}.

We have shown that the electric-field-control of the spin-resolved frontier energy levels of the isolated graphene diamond nanofragments we recently predicted remains intact when the spin-polarized graphene diamond is coupled to metallic graphene ribbons. These calculations suggest a spin-polarized FET device which allows for very-large integration within a single graphene sheet and which has the potential to be the basis for an all-carbon spintronics. Electronic-transport calculations of the device show that conductance and the rate of spin-current polarization of the FET device can be selectively tuned by the application of a *gate* electric field.

Acknowledgments

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References and Notes

1. Du X, Skachko I, Barker A, Andrei EY. *Nature Nanotechnology* 2008;3:491.
2. Bolotin KI, Sikes KJ, Jiang Z, Klima M, Fudenberg G, Hone J, Kim P, Stormer HL. *Solid State Communications* 2008;146:351.
3. Lee C, Wei X, Kysar JW, Hone J. *Science* 2008;321:385. [PubMed: 18635798]
4. Seol JH, Jo I, Moore AL, Lindsay L, Aitken ZH, Pettes MT, Li X, Yao Z, Huang R, Broido D, Mingo N, Ruoff RS, Shi L. *Science* 2010;328:213. [PubMed: 20378814]
5. Westervelt RM. *Science* 2008;324. [PubMed: 18420920]
6. Ihn T, Güttinger J, Molitor F, Schnez S, Schurtenberger E, Jacobsen A, Hellmüller S, Frey T, Dröscher S, Stampfer C, Ensslin K. *Materials Today* 2010;13:44.
7. Ponomarenko LA, Schedin F, Katsnelson MI, Yang R, Hill EW, Novoselov KS, Geim AK. *Science* 2008;320:356. [PubMed: 18420930]
8. Lin YM, Dimitrakopoulos C, Jenkins KA, Farmer DB, Chiu HY, Grill A, Avouris P. *Science* 2010;327:662. [PubMed: 20133565]
9. Wimmer M, Akhmerov AR, Guinea F. *Physical Review B* 2010;82:045409.
10. Fernandez-Rossier J, Palacios JJ. *Physical Review Letters* 2007;99
11. Wang WL, Meng S, Kaxiras E. *Nano Letters* 2008;8:241. [PubMed: 18052302]
12. Agapito LA, Kioussis N, Kaxiras E. *Physical Review B* 2010;82:201411.
13. Bai J, Cheng R, Xiu F, Liao L, Wang M, Shailos A, Wang KL, Huang Y, Duan X. *Nat Nano*. 2010 advance online publication.
14. Han MY, Özyilmaz B, Zhang Y, Kim P. *Physical Review Letters* 2007;98:206805. [PubMed: 17677729]
15. Chen Z, Lin YM, Rooks MJ, Avouris P. *Physica E: Low-dimensional Systems and Nanostructures* 2007;40:228.
16. Blake P, Yang R, Morozov SV, Schedin F, Ponomarenko LA, Zhukov AA, Nair RR, Grigorieva IV, Novoselov KS, Geim AK. *Solid State Communications* 2009;149:1068.
17. Golizadeh-Mojarad R, Datta S. *Physical Review B* 2009;79:085410.
18. Mueller T, Xia F, Freitag M, Tsang J, Avouris P. *Physical Review B* 2009;79:245430.
19. Ryo N, Katsumi T. *Applied Physics Letters* 2010;96:253503.

20. Kim KS, Zhao Y, Jang H, Lee SY, Kim JM, Kim KS, Ahn JH, Kim P, Choi JY, Hong BH. *Nature* 2009;457:706. [PubMed: 19145232]
21. Jia X, Hofmann M, Meunier V, Sumpter BG, Campos-Delgado J, Romo-Herrera JM, Son H, Hsieh YP, Reina A, Kong J, Terrones M, Dresselhaus MS. *Science* 2009;323:1701. [PubMed: 19325109]
22. Girit CO, Meyer JC, Erni R, Rossell MD, Kisielowski C, Yang L, Park CH, Crommie MF, Cohen ML, Louie SG, Zettl A. *Science* 2009;323:1705. [PubMed: 19325110]
23. Campos-Delgado J, Romo-Herrera JM, Jia X, Cullen DA, Muramatsu H, Kim YA, Hayashi T, Ren Z, Smith DJ, Okuno Y, Ohba T, Kanoh H, Kaneko K, Endo M, Terrones H, Dresselhaus MS, Terrones M. *Nano Letters* 2008;8:2773. [PubMed: 18700805]
24. Lijie C, Li S, Deep J, Ana Laura E, Wei G, Mauricio T, Pulickel MA. *Advanced Materials* 2009;21:4487.
25. Campos LC, Manfrinato VR, Sanchez-Yamagishi JD, Kong J, Jarillo-Herrero P. *Nano Letters* 2009;9:2600. [PubMed: 19527022]
26. Soler JM, Artacho E, Gale JD, Garcia A, Junquera J, Ordejon P, Sanchez-Portal D. *Journal of Physics-Condensed Matter* 2002;14:2745.
27. Perdew JP, Burke K, Ernzerhof M. *Physical Review Letters* 1996;77:3865. [PubMed: 10062328]
28. Ohta T, Bostwick A, Seyller T, Horn K, Rotenberg E. *Science* 2006;313:951. [PubMed: 16917057]
29. Nakada K, Fujita M, Dresselhaus G, Dresselhaus MS. *Physical Review B* 1996;54:17954.
30. Kim WY, Kim KS. *Nature Nanotechnology* 2008;3:408.
31. Muñoz-Rojas F, Fernández-Rossier J, Palacios JJ. *Physical Review Letters* 2009;102:136810. [PubMed: 19392393]
32. Son YW, Cohen ML, Louie SG. *Physical Review Letters* 2006;97
33. Koskinen P, Malola S, Hakkinen H. *Physical Review Letters* 2008;101
34. Wassmann T, Seitsonen AP, Saitta AM, Lazzeri M, Mauri F. *Physical Review Letters* 2008;101:096402. [PubMed: 18851629]
35. Koskinen P, Malola S, Hakkinen H. *Physical Review B*. 2009
36. Chuvilin A, Meyer JC, Algara-Siller G, Kaiser U. *New Journal of Physics* 2009;11:083019.
37. Lee GD, Wang CZ, Yoon E, Hwang NM, Ho KM. *Physical Review B* 2010;81:195419.
38. Ryu S, Han MY, Maultzsch J, Heinz TF, Kim P, Steigerwald ML, Brus LE. *Nano Letters* 2008;8:4597. [PubMed: 19053793]
39. Xie L, Jiao L, Dai H. *Journal of the American Chemical Society* 2010;132:14751. [PubMed: 20923144]
40. Yang R, Zhang L, Wang Y, Shi Z, Shi D, Gao H, Wang E, Zhang G. *Advanced Materials* 2010;22:4014. [PubMed: 20683861]
41. Agapito LA, Cheng HP. *Journal of Physical Chemistry C* 2007;111:14266.
42. Agapito LA, Cao C, Cheng HP. *Physical Review B* 2008;78
43. Song LL, Zheng XH, Wang RL, Zeng Z. *The Journal of Physical Chemistry C* 2010;114:12145.
44. Zhang Y, Tang TT, Girit C, Hao Z, Martin MC, Zettl A, Crommie MF, Shen YR, Wang F. *Nature* 2009;459:820. [PubMed: 19516337]
45. Castro EV, Novoselov KS, Morozov SV, Peres NMR, dos Santos JMBL, Nilsson J, Guinea F, Geim AK, Neto AHC. *Physical Review Letters* 2007;99:216802. [PubMed: 18233240]
46. Son YW, Cohen ML, Louie SG. *Nature* 2006;444:347. [PubMed: 17108960]
47. Zeng MG, Shen L, Cai YQ, Sha ZD, Feng YP. *Applied Physics Letters* 2010;96:042104.
48. Furst JA, Brandbyge M, Jauho AP. arXiv:0909.1756v1. 2009
49. Wimmer M, Adagideli Ąn, Berber S, Tománek D, Richter K. *Physical Review Letters* 2008;100:177207. [PubMed: 18518334]
50. Ezawa M. *Physica E: Low-dimensional Systems and Nanostructures* 2009;42:703.
51. Yazyev OV, Katsnelson MI. *Physical Review Letters* 2008;100:047209. [PubMed: 18352331]
52. Ezawa M. *Physical Review B* 2007;76:245415.
53. Ezawa M. *New Journal of Physics* 2009;11:095005.
54. Ezawa M. *Physical Review B* 2009;79:241407.

55. Wang, Y.; Cao, C.; Cheng, HP. 2010. <http://arxiv.org/abs/1005.3075v1>
56. Cantele G, Lee YS, Ninno D, Marzari N. Nano Letters 2009;9:3425. [PubMed: 19731918]
57. Balog R, Jorgensen B, Nilsson L, Andersen M, Rienks E, Bianchi M, Fanetti M, Laegsgaard E, Baraldi A, Lizzit S, Sljivancanin Z, Besenbacher F, Hammer B, Pedersen TG, Hofmann P, Hornekaer L. Nat Mater 2010;9:315. [PubMed: 20228819]
58. Coletti C, Riedl C, Lee DS, Krauss B, Patthey L, von Klitzing K, Smet JH, Starke U. Physical Review B 2010;81:235401.

Figure 1.

(a), (b) Schematic of an all-carbon-electronics microchip, where all internal devices and interconnects are carved from a one-atom thick graphene sheet (shown in b) and foreign metals (yellow) are used only for the outmost contact pads (shown in a). (c) The device region of graphene-FET junction used for the transport calculations. It comprises of a $N=8$ graphene diamond nanofragment with hydrogenated zigzag edges interconnected to two semi-infinite non-hydrogenated (5,7)-reconstructed graphene nanoribbons. An external coplanar electric field F is used as a *control gate*. Blue, red, and white denote spin-up, spin-down, and absence of magnetization, respectively. For visualization the colorbar shows only a subset of the full range (from -0.3 to +0.3), in units of Bohr magneton.

Figure 2.

Total energies of the ferromagnetic (green) and nonmagnetic (red) configurations, relative to the antiferromagnetic (blue), versus the diamond size N for the isolated diamond graphene nanofragment. The inset shows the variation of the HOMO-LUMO gap for the AF configuration with diamond size.

Figure 3.

(a) Electric field modulation of the frontier energy levels for the AF state of the $N = 8$ isolated hydrogenated graphene diamond. The energy bandgap of the spin-up (spin-down) energies, shown in blue (red), decreases (increases) to its minimum (maximum) value of 40 (860) meV at $F = 0.23$ (0.14) V/Å. For higher field $F > 0.73$ V/Å the system undergoes a transition into a nonmagnetic state (NM). The vertical dashed lines indicates the fields corresponding to the bandgap minimum and the AF→NM transition. (b) Variation of the local magnetization of the AF-state $N=8$ diamond with electric fields (in V/Å), where the spin-up, spin-down, and absence of magnetization are denoted by blue, red and white, respectively. The electric field F is applied coplanar and parallel to the larger diagonal of the diamond, as seen in Figure 1c. For visualization the colorbar does not show the full range (from -0.3 to +0.3), in units of bohr magneton.

Figure 4.

(a) Zero-bias and zero-gate total electron transmission function, TF, for an infinite (5,7)-reconstructed carbon nanoribbon in the absence (green) and presence (black) of the $N=8$ graphene diamond scattering center, shown in Figure 1c. (b) Gate field variation of the spin-up (blue) and spin-down (red) transmission function of the $N=8$ graphene diamond coupled the (5,7)-reconstructed ribbon. The various thick blue curves denote the field-variation of the spin-up peaks of the HOMO, HOMO-1, LUMO, and LUMO+1, respectively, which have $TF=1$. For $F = 0$ and $F > 0.6 \text{ V/\AA}$ the spin-polarized TF peaks are degenerate, and are denoted in black.

Figure 5.

(a) Modulation of the total current ($I = I^\uparrow + I^\downarrow$) versus the gate field F for various bias values V_{bias} . (b) Current spin polarization, $\text{CSP} = (I^\uparrow - I^\downarrow)/(I^\uparrow + I^\downarrow) \times 100$, ratio as a function of gate field.