# Spintronic devices based on graphene nanoribbons with transition metal impurities. Towards space applications

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*"Any sufficiently advanced technology is indistinguishable from magic"* (*Clarke's third law*)

***Abstract:*** *Very recent publications draw the attention to a possible revolution that nanotechnology can cause in aviation. The effervescence in the peak field of nanomaterials is remarkable, as evidenced by the number of Nobel prizes recently awarded. A class of nanomaterials, the nanosensors, whose object of study is the present work, represents a special interest in space applications. More specifically, this article proposes the synthesis of a nanosensor based on active control and manipulation of spin degrees of freedom in the graphene nanoribbons (GNR), the strongest known substance. Thus, the physical model, a GNR, is electrically connected to two electrodes. Different variations of Mn (Manganese) impurities in graphene, with the spins having preset configurations, are considered. When a magnetic field is detected, their spin change causing changes in the total energy and hence the variation of transmission function. Therefore, the concept of active control, which originated in the flight control and structural vibration problems, is naturally extended herein to the nanosensors synthesis. The used physico-mathematical model to determine the spin transport and the transmission function is based on density functional theory, Kohn-Sham equations and the SIESTA package. The differences between distinct GNR excited states were determined and it was established that the energy range overlaps the mid-infrared wavelengths. Therefore, structures of this kind may serve in spatial applications which exploit the infrared atmospheric window.*

***Key Words:*** *nanomaterials, nanosensors, graphene nanoribbons (GNR), spintronics, active control, Schrödinger equation, density functional theory (DFT), SIESTA package.*

## 1. INTRODUCTION

In the recent years, the materials science in top areas such as nanoscience and nanotechnology, witnessed a frenetic development. The Greek word *nanos* means "dwarf". In the context, "nano" refers to $10^{-9}$ physical dimension of length − the nanometer (nm), which is on the scale of atomic diameters. Thus, the nanoscience is in fact the study of atoms and molecules, whose size is on the nanometer scale ($1 \div 100$ nm). Therefore, these fields of theoretical and applied research intersect the quantum mechanics. Without excluding adjacent areas, INCAS Bulletin is programmatically quartered in the aerospace field. It is thus the purpose of this paper to draw the reader's attention to unexpected, at first sight, connections. Here's an article

published several years ago in a prestigious journal, [1], which refers to a new direction of research launched by European Space Agency (ESA) and lead by Office National d'Études et de Recherches Aérospatiales (ONERA): *the Space study using the quantum mechanics*.
The following five relevant fields were selected: 1) atomic clocks; 2) atomic inertial sensors; 3) detectors of law temperature and magnetic flux with an energy sensitivity unequalled by any other device; 4) superfluidity or quantum transition; 5) advanced nanodevices based using state-of-the-art semiconductor technology. At least two of the listed objectives come in touch with topics such as nanomaterials and spintronics.

We introduce two notions included in the title of the article: graphene nanoribbons (GNR) and spintronic devices.

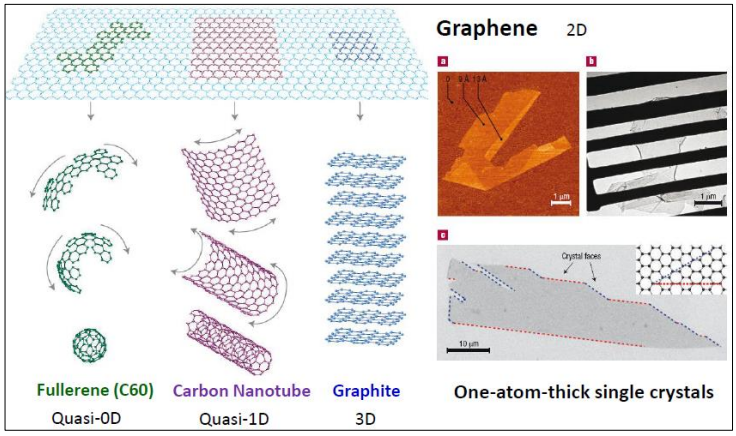



Fig. 1 Carbon materials ─ graphitic forms ─of various dimensionalities: wrapped up into 0D buckyballs, rolled into 1D nanotubes, stacked into 3D graphite. Graphene is the 2D building material [2], [3].

In 2010, the winners of the Nobel Prize in Physics *"for groundbreaking experiments regarding the two-dimensional material graphene"* became two researchers from the University of Manchester (UK), Andre Geim and Konstantin Novoselov. The graphene is a downright miraculous material, the thinnest of all materials in the Universe. The carbon atoms of graphene are arranged in two dimensional *"nanoribbons"*, making them the strongest substance known so far: it is 100 times tougher than the strongest steel and several times stiffer than diamond.

Such a ribbon could support the weight of an elephant, even even if it pressed the foil from an area equal to a pencil. Despite its strength, the graphene is extremely flexible and can be stretched to 120% of the surface without damaging it. Other graphene's superlatives [2]: record thermal conductivity (outperforming diamond); highest current density ar room temperature (106 times of copper); completely impermeable (even he cannot squeeze through); highest intrinsic mobility (100 times more than in Si); conducts electricity in the limit of no electrons; lightest charge carriers (zero rest mass).

As for natural resources, the raw material (the graphite) is found in abundance in the mines in Chile, India and Canada.

Technically, the graphene nanoribbon (GNR) is "a flat monolayer of carbon atoms tightly packed into a two-dimensional (2D graphite) honeycomb lattice, and is a basic building block for graphitic materials of all other dimensionalities. It can be wrapped up into 0D fullerenes, rolled into 1D nanotubes or stacked into 3D graphite" [2] (Fig. 1). It should be added that in 1985 the fullerenes have been discovered, the third allotrope of carbon (after diamond and graphite), in which the atoms form C60 molecules in the shape of a football. This led to the

award of the 1996 Nobel Prize in Chemistry to Harry Kroto (University of Sussex, Brighton, UK), Robert Curl and Richard Smalley (Rice University, Houston, USA), *"for their discovery of fullerenes"*. Currently, the fullerenes are seen as promising components of micro-electromechanical systems (MEMS) and, generally, in nanotechnology applications.

The technologies of manufacturing the graphenes, based on physics and chemistry [2], are put in place since 2004.

The potential applications of GNR relates to: integrated circuits, chemistry (redox), energy storage, thermal management, piezoelectricity, quantum dots, spintronics, medicine, biodevices, aerospace [4], [5].

*Spintronics*, or *spin transport electronics*, means the *active control* and manipulation of spin degrees of freedom in solid-state systems. The term *transport* refers to the transport of electrons in crystalline materials. Transport (or kinetic) phenomena are the orderly movement of charge carriers in response to the application of an electric field $\boldsymbol{E}$ (a current occurs), the application of a magnetic field $\boldsymbol{B}$ (Hall's effect) or a temperature gradient $\nabla T$ (Seebeck effect). Herein, the concept of transport involves properties such as electrical conductivity, energy band etc. In spin-polarized metals, various characteristics remain to be tuned, as will be seen in Section 5, using the spin as key element.

It is known that the experiment conducted in 1922 by Stern and Gerlach has founded the principles of quantum mechanics, and led to the Pauli's theory of electron spin as a tiny intrinsic discrete amount of angular momentum, equal to $1/2$.

The magnetic properties of GNR with certain edge geometries have received much attention due to possible applications [6], [7], *as magnetic nanosensors*, for example. The studies show, however, that the magnetic properties of a pristine GNR are not robust in the presence of edge disorder. These properties have become more interesting and more robust in the case of some metal impurities properly distributed in GNR with various geometries edge; armchair and zigzag types are taken in [8]. In the present paper, as in most recent works in the field, an efficient mathematical approach to the Schrödinger equation is used, *Density Functional Theory* (DFT), having as precursor Thomas-Fermi approximation [9] and whose foundations are given in [10], [11]. The DFT technique, which includes specific procedures, for example Kohn-Sham band structures [10], is implemented in the free specialized package SIESTA [12], [13], a code for *ab-initio* electronic structure and molecular dynamics simulations [13]. SIESTA is the acronym for *the Spanish Initiative for Electronic Simulations with Thousands of Atoms*. We add that Walter Kohn was awarded with the Nobel Prize in Chemistry in 1998 for his development of DFT.

In this paper, a GNR is electrically connected to two electrodes. Different variations of Mn (Manganese) impurities in graphene, with the spins having preset configurations, are considered. When a magnetic field is detected, their spin change causing changes in the total energy and hence the variation of transmission function. Therefore, the concept of active control, which originated in the flight control and structural vibration problems [14], [15], herein is naturally extended to the *nanosensors synthesis*. The used physico-mathematical model to determine the spin transport and the transmission function is based on DFT, Kohn-Sham equations [11] and the SIESTA package.

The article is organized as follows. The physical model of a magnetic nanosensor based on spin filtering in GNR with Mn impurities is presented in Section 2. The associated mathematical model is briefly described in Section 3. The presentation reviews the transition from the Schrödinger equation model, unrealistic in computer applications, to the DFT methodology. This mathematical construction served as theoretical framework for a computer program, the SIESTA package, detailed in Section 4. Based on various runs on SIESTA

package, Section 5 discusses the results of active control and spin manipulation in view of GNR nanosensor synthesis. Concluding remarks of the work are presented in Section 6.

## 2. DEVELOPING A NANOSENSOR BASED ON SPIN FILTERING IN GNR WITH Mn IMPURITIES

The origins of the nanostructures are found in the allotropes of carbon: graphite, C60 or Buckminsterfullerene, single-walled carbon nanotubes. The graphite is made by many layers of graphene which is a two-dimensional honeycomb grid formed with carbon atoms in the $sp^2$ hybridization form (the chemical bonds between carbon atoms are situated in plan and the angle between two carbon-carbon bonds is equal to 120º) [16]. The graphene represents a promising material for spintronics applications due to the low spin-orbital interactions [17, 18]. To use it in technology, this is cut in a quasi-one-dimensional structure with a width smaller than 10 nm [19]. The structure is labeled as *graphene nanoribbon* (GNR).

For a better understanding of the notions that will be presented, it is necessary to make a brief overview of the spin. In quantum mechanics, the *spin* is defined as the intrinsic form of the angular momentum for an elementary particle (which cannot be divided in smaller unities). The spin has a direction (a little different from an ordinary vector) and a magnitude. An elementary particle cannot be made to spin slower or faster. The SI unit of the spin is the joule-second. The spin is independent of the particle spatial degrees of freedom [20].

Every elementary particle has a given spin quantum number. Mathematically, the spin quantum number is described by the formula $s = n/2$, with $n$ non-negative integer. The particles with half-integer spins are known as *fermions*. Fermions include electrons and protons. The *bosons* are those particles with integer spin. Hence, the *phonons* (quarks, leptons etc.) are part of this class. It can be seen that the value of the spin gives different properties [21]. The electrons are fermions with spin 1/2. For this reason they obey the *Pauli's exclusion principle*: a particle can be found in a spin-up state or a spin-down state, it cannot exist in both spin-up-spin-down states simultaneously. That means the wave function for fermions is anti-symmetric [22].

Spatial distribution of particles by spin orientation can be ferromagnetic (FM) or antiferromagnetic (AFM). A FM structure refers to the fact that all particles have the same spin direction: spin-up or spin-down. In the AFM distribution, the direction of spin varies: spin-up followed by spin-down, than spin-up again and so on as can be seen in Fig. 2.

Geometrically, there are only two possible nanoribbons categories: those with *zigzag edge* (zGNR) or an *armchair edge* (aGNR) [23, 24, 6]. *The edge and the width of the graphene have a significantly impact on the electronic properties of the nanoribbon* [25]. The *ground state* of a quantum mechanical system is its lowest-energy state. An excited state is any state with energy greater than the ground state. At the ground state all graphene nanoribbons are semiconductors [26]. All zigzag GNRs with the two edges coupled FM are metallic, while the conductor character of armchair GNRs depends on its width [8].

*Pristine graphene is nonmagnetic*. Graphene nanoribbon presents spin polarization on the two edges. *Based on spin polarization control on the edges by applying an electric field* [25] *or a magnetic field* [6], *the nanoribbons can be used for spintronics applications*. To induce magnetism in a nonmagnetic material like the graphene, a *method of doping with transition metals* (elements located in d-block of the periodic table with partially filled d sub-shell) is used [27]. These are adsorbed as interstitial impurities or are embedded in vacancies [7]. The

electric and magnetic properties of the nanoribbon are affected by the direction of spin from the edges (FM or AFM).

Also, the impurities in the scattering area influence the current flow through the nanodevices; so, *the nanoribbon can be used as a tunnable spin filter, which is the basic building block for the nanosensor*.

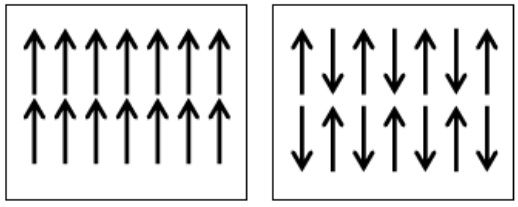



Fig. 2 Spatial distribution of particles by spin orientation: a) ferromagnetic (FM); b) antiferromagnetic (AFM).

In our setup spin filtering effects of Mn-doped zigzag graphene nanoribbon was analyzed. The scattering region is made of four unit cells with 50 carbon atoms and 10 hydrogen atoms and is connected to zigzag graphene nanoribbon electrodes as can be seen in Fig. 3. The scattering region and the electrodes have the same structure. The zGNR in the FM edge configuration was used due to its metallic character. Four Mn atoms as magnetic impurities were introduced.

The impurities substitute carbon atoms localized at the hydrogen passivated edges. The ground state density and total energy are calculated using the density functional theory (DFT) included in the SIESTA package using Ceperly-Alder parametrization in the local spin density approximation (LSDA).

The transmission functions are calculated using the non-equilibrium Green's functions (NEGF) formalism included in TranSIESTA [28]. The total transmission function corresponding to a total energy E is given by $T(E)=Tr[\Gamma_L G^r \Gamma_R G^a]$, where $G^r$, $G^a$ are the advanced, respectively retarded, Green's functions and $\Gamma_L$, $\Gamma_R$ are the self-energies corresponding to the coupling between the scattering region and the two electrodes [29].

The polarization of the spin current gives the efficiency of our spin-filtering nanosensor using the relation: $p = (T_\uparrow - T_\downarrow)/(T_\uparrow + T_\downarrow)$ [30].

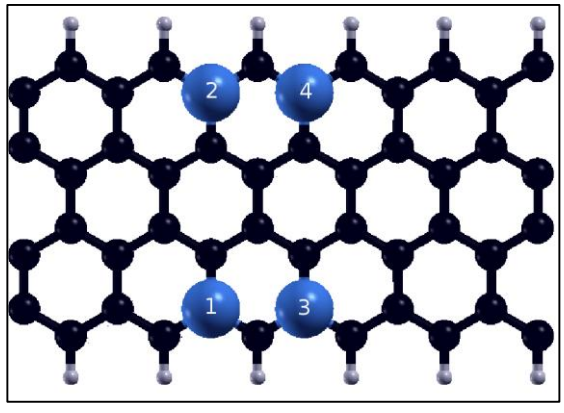



Fig. 3 The device structure: graphene nanoribbon with hydrogen passivated edges and four Mn impurities.

## 3. MATHEMATICAL MODELING

As stated in Section 1, the mathematical model for the spin transport and the transmission function of GNR physical models considered in Section 2 is based on DFT and Kohn-Sham equations. These are efficient approaches for the solutions of the Schrödinger equation, which is far from a realistic model in solving practical problems. To be herein a self-contained text, remember that any problem of quantum mechanics starts with the necessity of solving the Schrödinger equation, which gives the ground state and excited states of a collection of atoms. In the time independent, nonrelativistic framework, the Born-Oppenheimer approximation of the Schrödinger equation is

$$\hat{H}\Psi\left(r_1, r_2, ..., r_N\right) = E\Psi\left(r_1, r_2, ..., r_N\right) \tag{1}$$

The Hamiltonian $\hat{H}$ is a notation for the system's energy operator, and consists of the kinetic energy, the interaction with the external potential (*V*ext) and the electron-electron interaction (*V*ee) ( $r_i$ is the coordinate of the electron *i*)

$$\hat{H} = -\frac{1}{2}\sum_{i}^{N}\nabla_i^2 + \hat{V}_{\text{ext}} + \sum_{i<j}^{N}\frac{1}{\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|} \tag{2}$$

$\Psi$ is the notation the *state function*, also called the *wave function* of the considered quantum mechanical system, in fact an *eigenfunction* or *solution* of the equation (1). This function depending on the coordinates of the particle(s) and on the time, is subject to the constraint to be an antisymmetric function (it changes sign if the coordinates of two electrons are interchanged).

*In the Born interpretation,* $\Psi$ *is the probability density* $\Psi^*\left(r,t\right)\Psi^*\left(r,t\right)d\tau$ *to find the particle in the volume element* $d\tau = drdt$ *located at* ***r*** *at time t*. The average total energy for a state $\Psi$ is given as

$$E\left[\Psi\right] = \int \Psi^* \hat{\boldsymbol{H}}\, \Psi d\boldsymbol{r} \tag{3}$$

A variational theorem shows that the system's energy, a functional of $\Psi$, is higher than that of the ground state $\Psi_0$, $E\left[\Psi\right] \geq E_0$. This was used as searching criterion for approximate solutions $\Psi_{app}$. Such methods for molecular calculations, developed until the early 1980s, have been shown unrealistic [31]. The initiatives to find other approaches led to the famous DFT.

The main idea of DFT is to describe an interacting system of fermions [32] via its *density* and not via its many-body wave function $\Psi$. For *N* electrons in a solid, which obey the Pauli principle and repulse each other via the Coulomb potential, this means that the basic variable of the system depends only on three – the spatial coordinates *x*, *y*, and *z* – rather than 3*N* degrees of freedom [33].

The *density matrix* is the quantum-mechanical analogue to a phase-space probability measure (probability distribution of position and momentum) in classical statistical mechanics.

Thus, suppose a quantum system may be found in state $\Psi_1$ (for simplicity of writting, we evade the Dirac notation for ket vectors) of with probability $p_1$, or it may be found in state $\Psi_2$ with probability $p_2$, and so on. The density for this system is [34]

$$\rho(\boldsymbol{r}) = \sum_i p_i \left|\psi_i(\boldsymbol{r})\right|^2 \tag{4}$$

In the terminology of the field, $p_i$ is also called occupation numbers of the orbital $\Psi_1$. Also, the electron density is an *observable*, and the orbitals are just mathematical, but very efficient constructions.

The first Hohenberg-Kohn theorem [10] asserts that the density of any system determines all *ground-state* properties of the system, that is, $E = E[\rho]$, where ρ is the ground-state density of the system. The second Hohenberg-Kohn theorem shows that there exists a variational principle for the above energy density functional $E[\rho]$. Namely, if ρ' is not the ground state density of the above system, then $E[\rho'] > E[\rho]$. As shown, the theoretical results of DFT represent a mechanism parallel to that of the classical theory based on wave functions.

It should be added that in Kohn-Sham (KS) approach, the electrons are treated as *N* fictitious non-interacting particles moving in an effective potential. Consider $\Psi_i$ independent particle wave functions.

One can show that the $\rho_{KS}$ density is equal to the true system density. Thus, the obtained Kohn-Sham (KS) equation (Fig. 4) is finally the Schrödinger equation of a fictitious KS system of non-interacting particles (typically electrons) that generate the same density as any given system of interacting particles.

## 4. SHORT DESCRIPTION OF THE SIESTA PACKAGE

In our experimental simulation on the nanosensor consisting in a GNR with manganese impurities we used SIESTA package. This is a computer program based on a self-consistent density functional theory (DFT) method which calculates the electronic structure and is able to simulate molecular dynamics.

This method uses a standard norm-conserving pseudo potentials and a numerical linear combination of atomic orbitals basis set [35].

The Kohn-Sham equations are numerically solved for all the electrons in the system in an iterative mode. Every iteration changes the electronic configuration.

For optimizing the program, the deep core electrons are eliminated while the valence electrons are included [35].

SIESTA is an N-order method, which means that the computational time scales linearly with the size of the system. For calculating the Hartree and exchange-correlation potentials and matrix elements, a localized basis is chosen.

SIESTA makes use of pseudo potentials that replace the potentials due to nuclei and core electrons. It uses a supercell setup, where periodic boundary conditions are imposed on all three directions.

Using the SIESTA program one can calculate: total and partial energy, electron density, atomic forces, stress tensor and one can perform spin polarized calculations [36]. Also, SIESTA contains a module named TranSIESTA which implements ballistic transport of electrons [28].

The method is based on non-equilibrium Green's functions (NEGF). Starting from a given electron density and using density functional theory in a self-consistent algorithm the non-equilibrium Green's functions are obtained and the transmission functions are determined [30].

The self-consistent algorithm of DFT consists in finding the solution of Kohn-Sham equation in an iterative mode. Starting from an initial density $\rho_i$ (see the relation (4)), the

effective potential formed by the external, Hartree and exchange-correlation potentials is calculated [37].

The next step is to introduce the new potential in the Kohn-Sham equation and to find the solution which will give a new density $\rho_f$.

The difference between the two densities is calculated. If the maximum of the difference is smaller than a tolerance parameter, the other properties of the nanostructure like energy, charge density and so on can be determined, else the self-consistent algorithm is reiterated, mixing the density matrices as presented in Fig. 4.

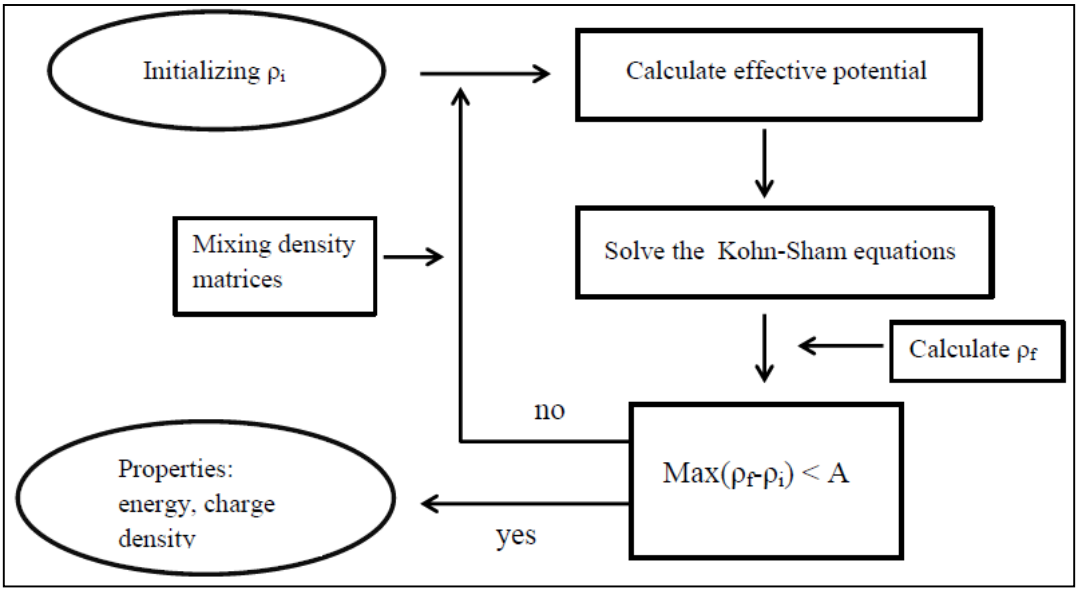



Fig. 4. Proposed in the paper self-consistent algorithm in the framework of DFT.

## 5. RESULTS AND DISCUSSION

The active element of the spintronic device is a zig-zag graphene nanoribbon (GNR) with four substitutional Mn impurities, placed near the edges, as depicted in Fig. 3. The transition metal impurities have incomplete *d*-shells and therefore possess net magnetic moment.

Similar devices based on hybrid BNC materials [17, 30], with one or two transition metal impurities indicate enhanced spin filtering properties. The transport in these devices is largely influenced by the edge states, which are spin polarized. In the case of pristine graphene nanoribbons the spin polarization of the two edges is anti-ferromagnetic in the ground state.

However, it is also possible to change the relative polarization of the edges by applying in-plane electric fields or by defect engineering. A GNR with ferromagnetic configuration of the two edges is metallic.

A first step of the numerical study was to evaluate the GNR the changes in the transmission functions introduced by different spin configurations of the Mn impurities.

The ab initio calculations are performed using the density functional theory (DFT) in the local density approximation (LDA) proposed by Ceperley and Alder [38], implemented by SIESTA [13]. It uses localized basis sets, which is key to obtain a linear scaling of the computational time with the problem size.

The GNR with ferromagnetic spin ordering at the edges is metallic as shown above. The difference obtained between the FM and AFM configurations is rather small, at about ~56

meV. The total energies – extracted for each spin configuration, with respect to the ground state – are indicated in Table 1.

Due to symmetry reasons one should notice that some of the spin configurations are equivalent. The ground-state of the system is obtained for the "+−+−" configuration or, equivalently, "−+−+" configuration, i.e. the Mn atoms are coupled ferromagnetically at short distance at each edge.

Between the two edges, the pairs of spins are coupled anti-ferromagnetically. The all-spins-up configuration "++++" as well as the all-spins-down configuration "−−−−" have the closest energies to the ground state at ~110 meV and ~102 meV, respectively. This is due to the fact that the interactions between spins 1 and 3, on one hand and 2 and 4 on the other hand, are dominant.

The other configurations assume at least one pair of spins at a certain edge with AFM coupling, which raises the energy of the system. The largest energy difference compared to the ground state, ~505 meV, is found for the "++−−", "−−++" configurations, for which both pairs of spins at the two edges are coupled AFM.

A second step of the numerical study was to analyze a typical spin-transfer characteristics that presented in Fig. 5. The transmission functions for each spin component are calculated within the non-equilibrium Green's functions formalism. In the case of pristine GNR, the transmission functions indicate a series of steps, which correspond to individual channels which propagate with nearly perfect transmission. By contrast, introducing the Mn impurities one obtains typically lower transmission functions due to increased scattering induced by impurities.

For the all-spins-down configuration presented in Fig. 2, we observe that the up-spin is poorly transmitted, while the down-spin transmission around the Fermi energy is significant. In this configuration, the Mn impurities scatter the conduction electron spins from the up-spin state to the down spin-state. Therefore, instead of the two peaks, which are visible for the pristine GNR, for each spin component, one obtains at roughly the same energies two peaks for the down-spin transmission.

This has another important consequence, namely, the spin current polarization approaches 100% in this case. The polarization of the Mn atoms and their neighbors is responsible for the spin scattering. Therefore, we plotted in Fig. 6 the pseudo-spin density in comparison with the pristine GNR.

For the other spin configurations, the transmissions at the Fermi energy are indicated in Table 1. One can make a mapping between the energies of spin configurations and the spin up/down transmissions. The spin current polarization may also be associated with a certain spin configuration. In this way one can detect and quantify the size of the perturbation. There are 7 non-equivalent spin states and, in this set of configurations, transitions may occur. The energy differences range between 100-500 meV, which corresponds to the mid-wavelength infrared range (2.5-12 μm).

This range overlaps well with the infrared atmospheric window, which is exploited in aviation for the detection of the aircraft infrared signature. Moreover, the infrared radiation in this range is able to pass directly to space without intermediate absorption and re-emission. This is very important from the point of view of remote sensing on satellites since these windows occur at the same wavelength as the Earth's radiation output.

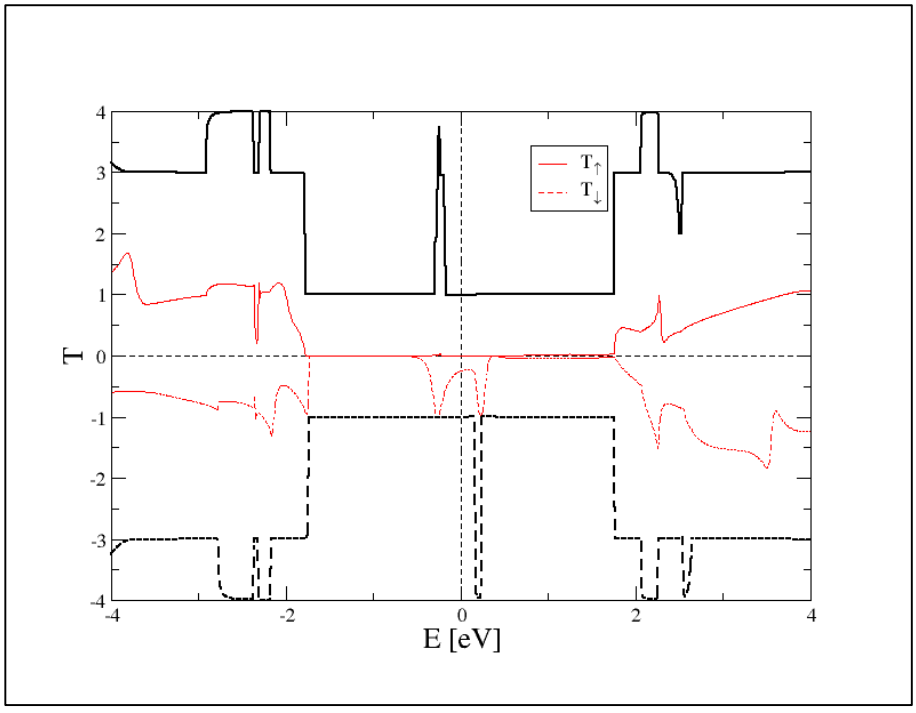
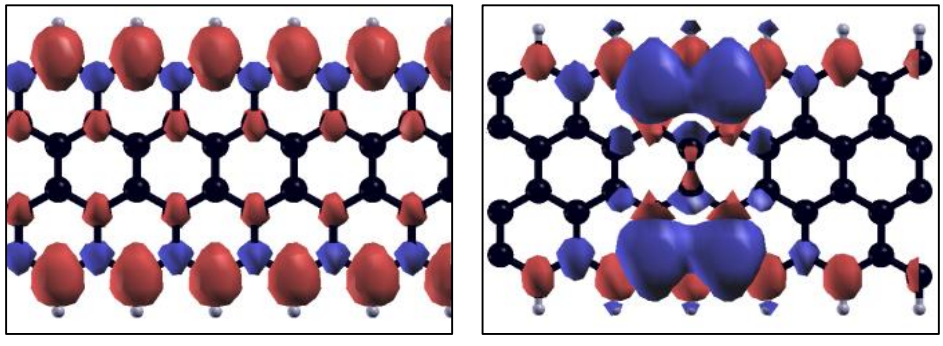



Fig. 5. Spin up/down transmission functions versus energy, for the pristine GNR (thick lines/black) and for the system with all-spins-down configuration (thin lines/red). The Fermi energy is marked by the vertical dashed line.

## 6. CONCLUSIONS

Spintronic devices based on graphene nanoribbons with transition metal impurities, with potential applications in mid-infrared sensing, were analyzed in the framework of spin constrained density functional theory calculations. The different spin configurations of the magnetic impurities were analyzed and their correspondence with the transmission coefficients was ascertained. The differences between different excited states were determined and it was established that the energy range overlaps the mid-infrared wavelengths.



a) b)

Fig. 6 Pseudo-spin density for the pristine GNR (a) and for the system with Mn impurities, in the all-spins-down configuration (b)

Table 1 Total energies [meV] with respect to the ground states "+−+−", "−+−+", transmission coefficients at the Fermi energy for up/down spin components and spin current polarization for different spin configurations.

| Spin configuration | +++−<br>++−+<br>+−++<br>−+++ | +−−−<br>−+−−<br>−−+−<br>−−−+ | ++−−<br>−−++ | +−+−<br>−+−+ | +−−+<br>−++− | ++++ | −−−− |
|---|---|---|---|---|---|---|---|
| Energy | 244 | 251 | 505 | 0 | 439 | 110 | 102 |
| $T_{\uparrow}$ | 0.53 | 0.25 | 0.16 | 0.80 | 0.51 | 0.17 | <0.01 |
| $T_{\downarrow}$ | 0.11 | 0.13 | 0.60 | 0.22 | 0.66 | 0.04 | 0.24 |
| p | 0.65 | 0.31 | −0.60 | 0.56 | −0.13 | 0.61 | <−0.92 |

*Therefore, structures of this kind may serve in spatial applications which exploit the infrared atmospheric window.*

This paper continues the research directions of the authors, focusing on areas such as the nanomaterials [39], the spintronics devices and the nanosensors [8], [17], [30], or belonging to interdisciplinary research directions, as the active control and the smart materials [14], [15].

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