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ARTICLE TYPE

Emergence of spin-filter states in Pt-Fe nanowires.

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Our theoretical study predicts the emergence of new *spin-filter* state in one-dimensional Pt-Fe bimetallic nanowires. The results show the existence of two transmission states in contracted "zig-zag" Pt-Fe nanowires with low and high transmission $1G_0$ and $3G_0$ correspondingly and one transmission state in linear stretched nanowires with conductance $2G_0$. Our first principle calculations revealed the dependence of quantum conductance of Pt-Fe nanowire on their geometry and atomic structure. Thus we found that nanowire stretching up to interatomic distance 2.3Å leads to the transition of the wire from "zig-zag" to the linear configuration leads to the changes of conductance properties of the wire, i.e. formation of new *spin-filter* state. Our study shows also the emergence of a magnetic transition from ferromagnetic to antiferromagnetic states under wire stretching. We found that the *spin-filter* state exists only in "zig-zag" Pt-Fe nanowires in ferromagnetic state. Moreover the spin-polarization of quantum electron transport through Pt-Fe nanowires vanishes totally in linear stretched nanowires in antiferromagnetic state. Our electronic structure calculation reveals the emergence of new hybridized states in band structure of the Pt-Fe nanowire that causes the formation of new *spin-filter* state.

Current development of electronics requires miniaturization of the base elements of the nanoschemes. One way to miniaturize the electronic devices is the development of new spintronic devices. Currently researchers in the field of spintronics are searching new conducting magnetic nanostructures. The electronic transport in these nanostructures may be spin-polarized which allows to significantly increase the data recording and transmission densities without increasing the size of nanostructures [1,2]. Spin-polarization of the electronic current allows controlling the spin of atoms and thus the conducting properties of nanostructures as a whole by means of external magnetic or electric fields. The recent progress in nanoelectronics leads to an extended experimental and theoretical study of spin-polarized electron transport in magnetic one-dimensional nanostructures – nanowires and nanocontacts [3,4,5]. The relationship between magnetic and transport properties of magnetic nanocontacts was first established in experimental work of Chopra et al. in 2002, it was called the "giant magnetoresistance" (GMR) [2]. The foundation of this new effect opens an avenue of controlling of magnetic and conductance properties of nanostructures. IBM's labs (Yorktown, New York) by using CMOS technology produced the first prototype of racetrack memory based on "giant magnetoresistance" in nickel nanowires. In 2006 Mokrousov et al. have predicted the emerging of giant magnetic anisotropy in freestanding metallic nanowires from 4d-elements [8]. However, the nanowires of magnetic material are not suitable elements for the construction of nanodevices because they are unstable and highly chemically reactive [5]. The absence of the magnetic properties in the most stable conducting nanocontacts (e.g. Au, Ag) at room temperatures motivated experimental and theoretical groups to study the quantum magnetic properties of mixed one-dimensional nanostructures. The work of Bettini et al. was the first successful experimental work on the formation of mixed Au-Ag nanocontacts at room temperature [9]. However, more useful for spintronics is the investigation of mixed nanocontacts consisting of low reactivity atoms of nonmagnetic transition and noble metals (Au, Pt, etc.) and atoms of magnetic elements (Co, Fe, Ni, etc.). Such mixed nanocontacts may possess an unusual magnetic properties (for instance, ballistic magnetoresistance) with high structural stability [6] and low chemical reactivity [7]. For the first time quasi-one dimensional nanocontacts from gold and cobalt atoms was obtained in the experimental work of Egle et al. [10]. They found the "giant magnetoresistance" (dependence of resistance of nanocontact on the direction of external magnetic field) in mixed Au/Co nanocontacts and its dependence on the chemical composition of the nanocontact. We have found the emergence of GMA (giant magnetic anisotropy) in Au-Co nanowires with the values of MAE (magnetic anisotropy energy) about 130meV per Co atom [11]. Our calculations also have shown that mixing of two types of atoms – atoms of magnetic elements (Fe, Co) and atoms of nonmagnetic late transition metals (Pd, Pt) or noble metals (Au) leads to formation of one-dimensional nanowires most stable to strain deformations of "stretching-contraction" with magnetic transition from ferromagnetic to an antiferromagnetic states under stretching of the nanowire [6]. The foundation of spin filter systems was the most important for spintronics. The first experimental demonstration of spin filtering

dates back to 1972, when Müller et al. found that electrons emitted from tungsten tips covered by Eu-S presented a high spin polarization of 89% [12] (the spin polarization is the percentage of spin-up electrons compared to the total number of electrons). Thus spin-filter emits electrons with predominantly one spin direction (spin-up or spin-down). The main topic of spintronics is the study of spin filtering properties of one dimensional nanostructures (nanowires and nanocontacts). The foundation of this new phenomenon in conducting magnetic nanowires opens an avenue for creation of principally new spintronics devices. In present work we report on the result of the theoretical study into the transport properties of freestanding magnetic mixed Pt-Fe nanowires.

The study of the magnetic properties of the mixed Pt-Fe nanowires was carried out using the program Vienna Ab-initio Simulation Package (VASP) which is based on the density functional theory (DFT) [13]. The calculations presented in this paper were based on the self-consistent Kohn-Sham equations [14]. Electronic states were described using the basis of plane waves [15]. The cutoff energy for plane wave basis of 250 eV was used. All calculations presented in this paper were performed using the generalized gradient approximation (GGA) and also local density approximation (LDA) for exchange-correlation functional and PAW (Projector Augmented-Wave) pseudopotentials (Perdew-Wang '91 treatment) [16,17]. A structural relaxation was performed via a quasi-Newton algorithm, using the exact Hellmann-Feynman forces acting on each atom [18]. The total energies of the system were converged up to 1 meV/atom, while the residual force acting on each atom was less than 0.01 eV/A. The integration over Brillouin Zone (BZ) was performed using the tetrahedron method with Blöchl corrections. To calculate the total energy of the system we carried out the integration in reciprocal space by a special *k*-points grid of 1 × 1 × 7 constructed according to *k*-point mesh in Monkhorst-Pack scheme [19]. The structure of mixed Pt-Fe nanowires (NWs) for magnetic calculations has been represented by means of three dimension supercell with periodic boundary conditions. Pt-Fe wire was represented by an atomic chain aligned along the *z* axis separated from its images along the *x* and *y* directions (~10Å) to avoid spurious interactions with them. A one-dimensional Brillouin zone was used, along the *z* axis of the wire. Mixed Pt-Fe nanowire was modeled as a four atomic chain of two Pt and two

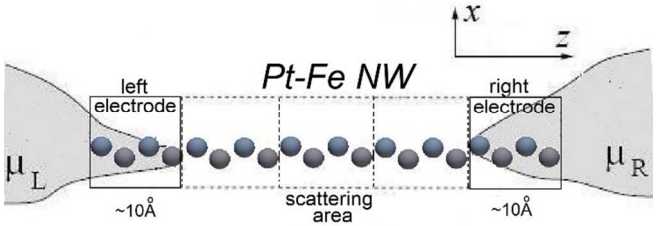

Fig. 1 Schematic illustration of the quantum transport problem through bimetallic nanowire.

Fe atoms, located along the *z* axis. To compare the calculated results for different bimetallic NWs (areas of existence, transmission, energies, etc.) for stretched or contracted mixed NWs, we consider them as the functions of an average interatomic distance. Average interatomic distance (*d*) for bimetallic NW represents the sum of all bond lengths in the wire projected on the wire axis (*z* axis) divided by the number of atoms in the wire.

Transport calculations were carried out in the elastic limit, ballistic transport conductivity calculations were conducted within the Landauer–Buttiker formalism, where the (spin-dependent) conductance is given by (1) [20,21]

$$G_\sigma = \frac{e^2}{h}\sum_\sigma \sum_{ij} T_{ij}^\sigma = \frac{e^2}{h}\sum_\sigma T^\sigma(E) = \frac{e^2}{h}\sum_\sigma Tr[t_\sigma(E)t_\sigma^*(E)] = \frac{G_0}{2}\sum_\sigma T^\sigma(E) \quad (1)$$

where $\sum_{ij}$ indicates that the sum is performed over all channels at the Fermi energy (the open channels) and we have introduced the spin index σ (σ =↑, ↓). We can clearly see that the conductance is written in terms of the conductance quantum G_0. Most importantly we note that the conductance has been directly associated with the coefficients of the out-scattered wave functions of our simple problem. Hence the energy-dependent transmission probability has a form

$$T^\sigma(E) = Tr[t_\sigma(E)t_\sigma^*(E)] \quad (2)$$

Alternatively the scattering process can be described in terms of the scattering matrix, S, which relates the wavefunction of the incoming and outgoing electrons with respect to the step potential i. e., channels entering $|\Psi_{\text{in}}\rangle$ or leaving $|\Psi_{\text{out}}\rangle$ in the scattering region (Fig.1) correspond in our case bimetallic nanowire.

$$|\Psi_{in}\rangle = S|\Psi_{out}\rangle \quad (3)$$

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \quad (4)$$

and t and r are the transmission and reflection coefficients respectively for incoming waves from the left whereas t' and r' are the counter parts for incoming waves from the right. In the more general multi-channel problem r, t, r' and t' are matrices linked by equation

$$|t|^2 + |r|^2 = 1 \quad (5)$$

The NEGF(non-equilibrium Green function) formalism for transport calculation [22–26] combined with density-functional theory and implemented in SMEAGOL, [16–18] is used here to calculate the transmission coefficients. The retarded Green function for the extended nanowire from the Green function equation for Hamiltonain of right- or left-hand side electrodes $H_{R,L}$and overlap matrix $S_{MR,L}$ represent (6)

$$G_M^R(E) = [\epsilon^+ S_M - H_M - \Sigma_L^R(E) - \Sigma_R^R(E)]^{-1}, \quad (6)$$

$$\Sigma_{L,R}^R(E) = \left(\epsilon^+ S_{ML,R} - H_{ML,R}\right) G_{L,R}^{0R}(E) \left(\epsilon^+ S_{L,RM} - H_{L,RM}\right) \quad (7)$$

Moreover the $G_M^R(E)$ contains all the information about the electronic structure of the wire extended in the equilibrium with leads it can be directly used for extracting the zero-bias conductance G of the system (8)

$$G = \frac{2e^2}{h}\sum_{Tr}[\Gamma_L G_M^{R+}\Gamma_R G_M^R], \quad (8)$$

where transmission coefficients represented by (9)

$$T(E) = \mathrm{Tr}[\Gamma_L G_M^{R+}\Gamma_R G_M^R](E) \quad (9)$$

The CA (Ceperley/Alder) approximation (LDA) for the exchange-correlation potential is employed [27]. Troullier-Martins norm-conserving nonrelativistic and nonlocal pseudopotentials (PPs) are used for Fe and Pt. The atomic configurations for generating the PPs are $4s^2 3d^6$ (Fe) and $5d^{10}6s^0$ (Pt). The cutoff radii (in atomic units) for *s*, *p*, and *d* components of the pseudopotential generation are respectively 2.6 a.u., 2.73 a.u. and 2.6 a.u. for Pt and 2.35 a.u., 2.47 a.u. and 2.235 a.u. for Fe. The *ab initio* engine behind SMEAGOL is the numerical implementation of DFT contained in the SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) code [28,29] which uses finite-ranged numerical orbitals as basis set. Split-valence bases for Fe are of double zeta type for *s, p* and *d* orbitals with the largest cutoff radii being 6.0 a.u. The electronic temperature is 300K. A mesh cutoff of 250 Ry, which specifies the real-space grid for defining the potential and the electron density, is used.

Results and discussion

Present study of the Pt-Fe nanowires was motivated by our recent work on the quantum magnetic properties of Pd-Fe nanowires with the same electron configuration of the valence states which possess the magnetic transition from ferromagnetic into antiferromagnetic state under wire stretching [6]. Our theoretical study of atomic and electronic structure has shown that mixed Pt-Fe nanowires are stable in large area of interatomic distances (1.2Å- 2.6Å) and may possess a high structural stability at room temperature. As expected, we found a similar ferromagnetic transition in Pt-Fe nanowires at interatomic distance about 2.3Å accompanied by changes of geometry of the wire. Our *ab-initio* calculations have shown the transition of the Pt-Fe nanowire from linear configuration to a "zig-zag" one under wire contraction up to 2.3Å. We have calculated the conductance of magnetic Pt-Fe nanowires in the whole range of interatomic distances, corresponding to the area of bimetallic nanowire existence (1.2Å - 2.6Å). These calculations simulate the real processes taking place in the chain of mixed Pt-Fe nanocontact during its formation in experiment by using MKBJ [2] or STM [3,4] methods.

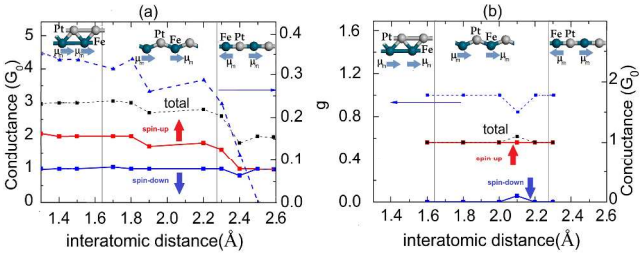

Fig. 2 Total quantum conductance of Pt-Fe nanowire (dotted line), spin-polarized conductance of spin-up (solid red line) and spin-down (solid blue line) channels and also the degree of spin polarization of quantum electron transport (g) as a function of average interatomic distance (dashed blue line): (a) "high transmission state", (b) "low transmission state".

Our study revealed the strong dependence of the total conductance of the wire on the "stretching-contraction" deformations emerging during the wire formation (see Fig.2, dotted line). The total transmission of linear stretched nanowires (with average interatomic distance >2.3Å) was calculated about $2.0G_0$ and remains practically unchanged in the range (2.3Å - 2.6Å) (Fig.2a, dotted line). Under contraction wire goes into "zig-zag" configuration at interatomic distance ~2.3Å. This structural transition of the wire leads to an abrupt increasing of transmission value to $3G_0$. Moreover our calculations revealed the emergence of a new "low transmission state" in "zig-zag" Pt-Fe nanowire with values of total transmission about $1G_0$ (Fig.2b, dotted line). Thus we found two transmission regimes in "zig-zag" Pt-Fe nanowire: "high transmission state" (Fig.2a) and "low transmission state" (Fig.2b) with unchanged conductance values into a range (1.6Å -2.3Å). Our total energy calculations have shown that the energy difference $\Delta E = E_{HTS} - E_{LTS}$ between energies of "low transmission state" (E_{LTS}) and "high transmission state" (E_{HTS}) of the wire changes under wire stretching or contraction. Table 1 shows the degree of "zig-zag" nanowire distortion (*x*) and values of energy difference ΔE for characteristic values of average interatomic distances (*d*) between atoms in nanowire. The energy difference ΔE is about zero in practically linear nanowires at average interatomic distances *d* ~2.3Å and this value increases significantly to ~1eV in strongly contracted nanowires at average interatomic distance *d*~1.6Å. The sign allows us to determine the ground state of the system. Our energy calculations have shown, that "low transmission state" is the ground state of the "zig-zag" Pt-Fe nanowire. In the stretched linear nanowires (>2.3Å) the ground state possesses the quantum transmission $2G_0$ and the "low transmission state" vanishes. Thus we have found the emergence of two way of electron transport into "zig-zag" bimetallic Pt-Fe nanowires with energy range depending on geometry of the wire.

Our electronic structure calculations have shown that spin-polarization of the Pt-Fe nanowire strongly depends on the geometry and also on the magnetic properties of the wire. By the fact that the main goal of spintronics is the search of systems with controllable spin of atoms, the next part of this work is devoted to the study of spin polarized electron transport of magnetic mixed Pt-Fe nanowires. Our study revealed the vanishing of spin polarization of electron transport in linear Pt-Fe nanowire, transmissions values through spin-up and spin-down channel are the same and equal $1G_0$ (see Fig.2, solid lines). These values of transmission through spin-up and spin-down channels remain unchanged in the range (2.3Å -2.6Å). Whereas the total conductance varies slightly, at the transition point drastically changes the magnetic characteristics of the current through the wire (current is spin-polarized in contracted wires and totally non spin-polarized in linear stretched nanowires). Similar changes of

current were observed in work of Nemnes et al. in graphen nanoribbons with magnetic impurities[30]. They found switching of two conductance regime and also emergence of spin filtering effects in Mn-dopped graphen nanoribbons by applying bias. For quantitative estimation of the spin polarization of the electron transport through nanowire, we introduce a term - degree of polarization [31]

$$g = \frac{G_\uparrow - G_\downarrow}{G_\uparrow + G_\downarrow} \qquad (10)$$

The value of g drastically decreases under wire stretching to ~0 for linear nanowire (Fig.2a, dashed line). It represents the vanishing of spin-polarization of electron transport in stretched bimetallic Pt-Fe nanowires.

To explain the emergence of new "low transmission states" we studied the dependence of ΔE on the geometry of the wire. For this purpose we have introduce the degree of the wire distortion in "zig-zag" configuration – *x*. Distances *x* represent the distance between Pt and Fe atoms in "zig-zag" nanowires perpendicular nanowire axis. At the Table 1 ΔE for some characteristic distances (*x* and *d*) are presented. The increasing of interatomic distance *x* leads to the decreasing of energy difference under strong nanowire contraction. The transition of bimetallic Pt-Fe nanowire to a system of interacting single component nanowires leads to the stabilization of "low transmission state" as ground state of the nanowire and vanishing of "high transmission state"(d~<1.6Å). Thus we found that two energy levels present only in "zig-zag" Pt-Fe nanowires. Stretched linear nanowires and system of two interacting Pt and Fe nanowires represent a one level system.

Table 1. Energy difference (ΔE) and deformation of bimetallic Pt-Fe nanowire (*x*) as a function of average interatomic distance *d*.

d(Å)	1.6	1.8	2.2	2.3
x(Å)	1.7	1.4	0.9	0
ΔE(eV)	0.942	0.153	0.216	0

Figure 3a illustrates the transmission spectra of the linear wire at interatomic distance 2.5Å. Our transmission spectra calculations have shown the absence of spin polarizations of electron transport in linear Pt-Fe nanowires. We can see that transmission through spin-up (red arrow) and spin-down (blue arrow) channels at Fermi level (Fermi energy of left and right electrodes) is identical and both about ~1G_0. Moreover our study of magnetic properties of the Pt-Fe wire has shown that stretched linear Pt-Fe nanowires are antiferromagnetic, thus antiferromagnetic ordering of spins of Fe atoms leads to the vanishing of spin-polarization of quantum electron transport through nanowire. Figure 3b illustrates the transmission spectra of "zig-zag" nanowire with average interatomic distance 2.2Å in "high transmission state". The value of transmission through spin-up channel is 2G_0 and through spin-down channel 1G_0 greatly differ from each other. The degree of spin polarization of electron transport (*g*) is about 0.33 (see Fig.2a, dashed line). This ratio remains practically unchanged in all range (1.5Å -2.3Å) corresponding to the area of "zig-zag" Pt-Fe nanowire existence.

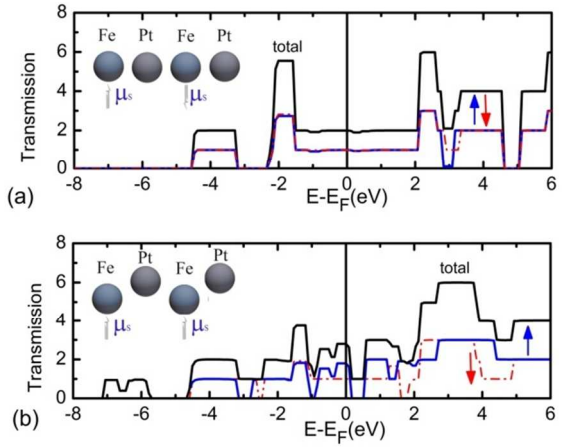

Fig. 3 Transmission $T(E)$ through spin-up and spin-down channel and total transmission at zero-bias of (a) linear Pt-Fe nanowire at average interatomic distance 2.5Å and (b) zig-zag nanowires at 2.2Å for ground state. E_F is the Fermi energy of left and right hand side electrodes.

The transmission pattern differs greatly for the mixed Pt-Fe nanowire in "low transmission state". Figure 4 illustrates the partial transmission through spin-up and spin-down channels for "low transmission state" (interatomic distance equals 2.2Å). We can see that only transmission through spin-up channel is presented at Fermi level (~1G_0), the transmission through spin-down channel equals zero. The degree of spin polarization (g) increases to 0.99 for nanowires in "low transmission state" (see Fig.2b, dashed line). Thus our transmission spectra calculations revealed that "low transmission state" of Pt-Fe nanowires represents the *spin-filter* system. Thus our study revealed the existence of two energy states of Pt-Fe nanowire with different types of conductivity: *spin filter* state ("low transmission state") and spin polarized state ("high transmission state") with energy

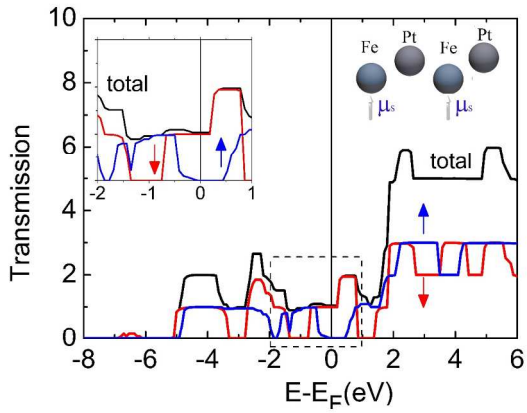

Fig.4 Transmission $T(E)$ of Pt-Fe nanowire at average interatomic distance 2.2 Å for "low transmission state"

difference (ΔE) depending on the interatomic distance of the wire.

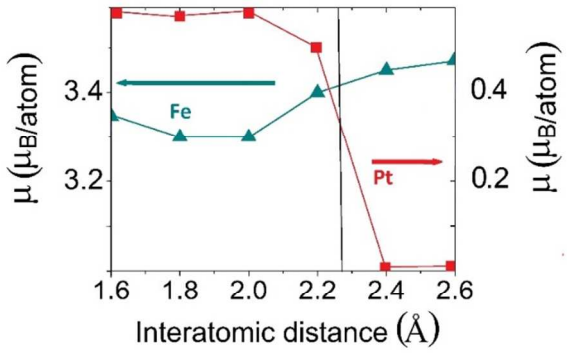

Fig. 5 The values of magnetic moments of Fe (rectangle) and Pt (squares) atoms as a function of interatomic distance.

Our calculation of magnetic properties of Pt-Fe nanowires have shown the strong correlation between transport and magnetic properties of the wires. We calculated the values of magnetic moments of Pt and Fe atoms of the wire in range of wire existence (1.2Å- 2.6Å). Figure 5 illustrates the dependence of local magnetic moments of Pt and Fe atoms on average interatomic distance in the wire. Our study revealed the slight changes of local magnetic moments of Fe atoms under "stretching-contraction" of the wire, however, the values of magnetic moments of Pt atoms depends significantly on the wire geometry (Fig.5). In contracted Pt-Fe nanowire magnetic moment of Pt atoms is about $0.6\mu_B$ which is in good agreement with our recent studies of magnetic properties of Pd and Pd-Fe nanowires[6,7]. However the magnetic moments of Pt atoms decreases drastically to $0\mu_B$ in linear stretched Pt-Fe nanowires in antiferromagnetic states. In antiferromagnetic linear nanowires Pt atoms are nonmagnetic which can lead to the vanishing of spin-polarization of the quantum current through the wire.

To explain the behavior of conductivity and also the magnetic properties of bimetallic Pt-Fe nanowires we present the study in detail of the band structures of bicomponent Pt-Fe nanowires in the next part of our work.

Our band structure calculations revealed the reason of the emergence of *spin filter* (low transmission) and spin-polarized (high transmission) states in the Pt-Fe wire. On Figure 6 the partial DOS of Pt-Fe nanowire in "zig-zag" configuration is presented. In the band structure of the Pt-Fe nanowire three hybridized bands are formed: d_{xy}-d_{x^2}, s-d_{z^2} and d_{xz}-d_{yz}. At the *spin filter* state ("low transmission state") (Fig.6b) only the d_{xz}-d_{yz} hybrid band formed at the Fermi level. This band makes a dominant contribution to the total density of states at the Fermi level. At the same time the contribution from other hybridized bands insignificant. New d_{xz}-d_{yz} hybrid band formed by the electron orbitals in the plane orthogonal to the wire axis as the result only one transmission channel formed and the total transmission of the Pt-Fe nanowire strongly decreases to the $1G_0$ with only one possible direction of spin of electrons according to Pauli principle.

Another band structure is observed in Pt-Fe nanowire in "high transmission state". (s-d_{z^2}),(d_{xz}-d_{yz}) and (d_{xy} –d_{x^2}) states of Fe atoms are placed at the Fermi level (Fig.6a). All these orbitals are strong hybridized with the same orbital of Pt atoms. As the result of strong band hybridization two half-filled states of Pt atoms are involved in the transmission process and both direction of spin of electron are possible. The dominate peak corresponds

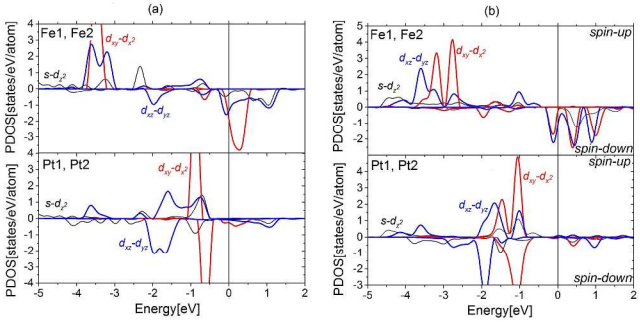

Fig. 6 Partial density of states for Fe and Pt atoms of the Pt-Fe "zig-zag" nanowire: (a) spin-polarized "high transmission state" and (b) *spin-filter* state ("low transmission state"). Average interatomic distance 2.2Å

to the (d_{xz}-d_{yz}) band. The weak peaks of (s-d_{z^2})- and (d_{xy} –d_{x^2})-bands are formed also at Fermi level. These three band form the three transmission channel.

The structure of orbitals and the type of hybridizations depend strongly on the geometry of the wire and external fields (interelectrodes voltage). In stretched Pt-Fe nanowire only s-d_{z^2} hybrid band is formed due to axial symmetry of the wire and *spin-filter* state doesn't form.

To explain the changes of magnetic properties of the wire and also the emergence of the ferromagnetic transmission under wire "stretching-contraction" we calculated the partial DOS of Pt-Fe nanowire at ferromagnetic and also antiferromagnetic states. Our band structure calculations have shown that the main impact in ferromagnetic transition has a (s-d_{z^2}) hybridized band. Figure 7 illustrates the structure of (s-d_{z^2}) hybridized bands of Pt and Fe atoms of the wire for contracted "zig-zag" nanowires in ferromagnetic state (Fig.7a) and also for stretched linear Pt-Fe nanowire in antiferromagnetic state (Fig.7b). Since the magnetic state of the Pt-Fe nanowires is determined by the relative orientation of magnetic moments of the Fe atoms, for clarity and convenience in describing of the results we introduced symbols Fe1 and Fe2 for the nearest iron atoms in the nanowire and Pt1 and Pt2 for the nearest platinum atoms (see inset figure on Fig.7). Figure 7a shows the partial DOS for (s-d_{z^2}) hybridized band of Pt and Fe atoms of the wire in the ferromagnetic state at the interatomic distance 2.2Å. The spin-up states of platinum atoms (Pt1, Pt2) (black line) overlap with the spin-up s-and d_{z^2}-states of iron atoms (Fe1, Fe2) (red line). The same situation occurs for spin-down states of iron (blue line) and platinum (Pt1, Pt2) (black

line) atoms. The spin up states of Pt and Fe atoms are completely filled, the spin-down state is partially filled. As a result, the magnetic moments of Pt and Fe atoms are non zero, moreover the spin-up states and spin-down states of iron atoms in the wire are

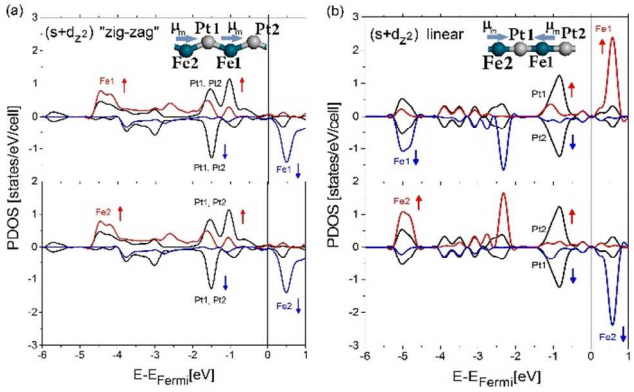

Fig.7 Partial DOSes for (*s*-d_{z^2})-states of Pt and Fe atoms in Pt-Fe nanowire (a) "zig-zag" nanowire at interatomic distance 2.2Å, (b) linear nanowire at interatomic distance 2.5Å.

strong correlated with each other. Due to the deviation of Pt and Fe atoms from the wire axis in "zig-zag" configuration a direct exchange interaction between Fe atoms appears in the wire, which stabilizes the ferromagnetic ordering into the Pt-Fe nanowires.

In the case of the antiferromagnetic ordering of iron atoms in linear wire the band structure of Pt-Fe nanowire varies strongly (Fig.7b). Figure 7b illustrates the partial density of (*s*-d_{z^2}) states in stretched linear Pt-Fe nanowires in the antiferromagnetic state at interatomic distance 2.5Å. Two intricate hybrid energy bands formed as a result of the overlapping of orbitals of Pt and Fe atoms: the first - formed by spin-down states of Pt2 (black line) and Fe1 (blue line) atoms, the second – by the spin-up states of Pt2 and Fe2 (red line) atoms (Fig.7b). Formation of this complex structure of hybrid zones in the wire leads to the emergence of the indirect exchange interaction[32] between the iron atoms through the states of platinum atoms, which leads to the formation of a stable antiferromagnetic solutions. The atoms of platinum "drag on" the electron density to the iron atoms on the partially filled (*s*-d_{z^2}) hybrid orbitals. The formation of the intricate hybrid bands in the Pt-Fe nanowire leads to the filling of the *d*-shell of Pt atoms and as result to the vanishing of local magnetic moments of Pt atoms.

A more detailed study of the electronic structure of "zig-zag" Pt-Fe nanowires showed that there arises an additional exchange interaction between the iron atoms (Fe1, Fe2) due to the formation of a new hybrid (d_{xz}-d_{yz}) and (d_{xy}-d_{r^2}) bands. In the contracted wire in "zig-zag" configuration the overlapping of these orbitals of iron atoms increases due to the deviation of the atoms from the wire axis and decreasing of average interatomic distance into the nanowire. The exchange interaction between the iron atoms in the wire increases, resulting in formation of a new hybrid energy bands. Direct exchange interaction between the iron atoms stabilizes ferromagnetic solution in contracted Pt-Fe nanowire. As a result, the ferromagnetic state becomes more energetically favorable in "zig-zag" nanowire. Besides the weakening of band hybridization between Pt and Fe atoms leads to the return of the charge from the Pt orbitals back to the Fe orbitals. The spin polarization of the Fe atoms decreases and also the values of local magnetic moments (Fig.5). After formation of two Pt and Fe nanowires under bimetallic nanowire contraction the electronic structure of the system drastically changes and the hybridized bands between Pt and Fe atoms vanish as the result the *spin-filter* state and antiferromagnetic ordering in the wire disappears totally, we obtain the transmission of Pt and Fe nanowires.

Conclusions

We found the emergence of new *spin-filter* state in one-dimensional Pt-Fe bimetallic nanowires. We revealed the effect of geometry and atomic structure of Pt-Fe nanowire on their conductance properties. Thus we found that formation of new *spin-filter* state is possible only in contracted "zig-zag" Pt-Fe nanowires. Moreover our calculations show the existence of two transmission states in contracted "zig-zag" Pt-Fe nanowires with low and high transmission $1G_0$ and $3G_0$ correspondingly and one transmission state in linear stretched nanowires with conductance $2G_0$. We found also the emergence of magnetic transition from ferromagnetic to antiferromagnetic states under wire stretching. Our *ab-inito* calculations show that the *spin-filter* state exists only in Pt-Fe nanowires in ferromagnetic state. Moreover the spin-polarization of quantum electron transport through Pt-Fe nanowires sustain only in ferromagnetic "zig-zag" nanowires and vanished totally in linear nanowires in antiferromagnetic state. As result of our band structure calculation we explain the formation of new *spin-filter* state in Pt-Fe nanowires.

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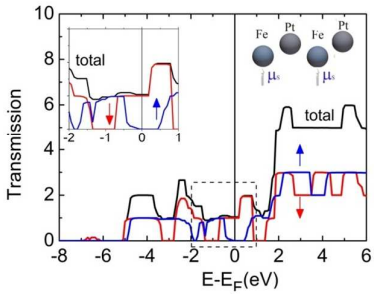

Our theoretical study predicts the emergence of new *spin-filter* state in one-dimensional Pt-Fe bimetallic nanowires.