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Symmetry Controlled Spin Polarized Conductance in Au Nanowires

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Abstract: The fact that the resistance of propagating electrons in solids depends on their spin orientation has led to a new field called spintronics. With the parallel advances in nanoscience, it is now possible to talk about nanospintronics. Many works have focused on the study of charge transport along nanosystems, such as carbon nanotubes, graphene nanoribbons, or metallic nanowires, and spin dependent transport properties at this scale may lead to new behaviors due to the manipulation of a small number of spins. Metal nanowires have been studied as electric contacts where atomic and molecular insertions can be constructed. Here we describe what might be considered the ultimate spin device, namely, a Au thin nanowire with one Co atom bridging its two sides. We show that this system has strong spin dependent transport properties and that its local symmetry can dramatically change them, leading to a significant spin polarized conductance.

1. Introduction

The field of spintronics, i.e., the simultaneous manipulation of charge and spin of the electron for the design of electronic devices, really had its starting point in the discovery of the giant magnetoresistance (GMR) effect,[1,2] which is now widely applied in magnetic reading heads. The use of the spin degrees of freedom in the past decade has also attracted the attention of the semiconductor community, with the findings of diluted magnetic semiconductors made from III−V materials,[3,4] and more recently a lot of research has also been dedicated to the study of spin injection[5–7] and spin coherence.[8–10] With the parallel advances in nanoscience and nanotechnology, it is now possible to talk about nanospintronics.[11] New behaviors will come up at this scale with the manipulation of a small number of spins,[12] such as for example the possibility of creating entangled states to perform quantum computation.[13] Another area where great advances have been made is the study of charge transport along nanosystems, such as carbon nanotubes,[14] graphene nanoribbons,[15,16] or metallic nanowires,[17] and spin dependent transport properties in such nanosystems may lead to new types of devices. In particular, metal nanowires (NWs) such as Au have been studied as electric contacts where atomic and molecular insertions can be constructed in order to emulate nanoscopic devices that use the electric charge as carriers. Another possibility is to consider magnetic insertions to be used as spin devices to operate in nanospintronics. Here we describe what might be considered the ultimate spin device, namely, a Au thin nanowire with one Co atom bridging its two sides. Using first principles density functional theory (DFT) electronic structure methods and nonequilibrium Green's function theory (NEGF-DFT) to calculate structural, electronic, and transport properties, we show that the insertion of a transition metal atom in a Au NW can result in strong spin dependent transport properties. In particular, the local symmetry of the nanowire can dramatically change these transport properties. We either observe Fano-like resonances if the symmetry permits the

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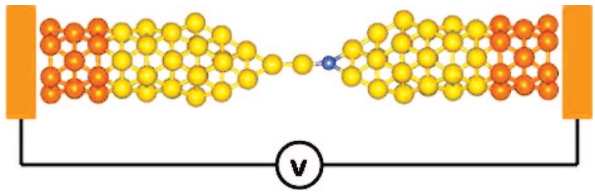

Figure 1. Scattering region used in the transport calculations, with the Au NW with Co. The darker atoms represent the bulk-like regions that couple to the left and right leads[42] (which are infinite repetitions of these dark-atom structures). All atoms except these darker ones were allowed to relax.

mixing between the nanowire s-orbitals and the Co d-states or a simple sum of independent transmission channels if the symmetry decouples such states. Moreover, depending on the local atomic arrangement we observe a significant spin polarized conductance. Thus, such a wire, if constructed, can be used as part of a spin device.

Experiments have studied a great number of molecules, atoms, and nanostructures attached to metallic terminations.[18–21] They include molecules probed in a two-terminal geometry of controlled break junctions[22] or scanning probes,[23] single molecule transistors made from carbon nanotubes,[19] and C-60 molecules.[24] With these available techniques it is possible to produce metallic constrictions in Au nanowires with a single atom separating the two leads. Attempts to produce electronics at the nanoscale have used largely metal nanowires. If these electronic features are associated to spin degrees of freedom, spintronics can also be studied in metal nanowires. For example, one can attach one Co atom to a Scanning Tunneling Microscope (STM) tip and touch a surface, and then upon drawing this tip from the sample, a nanowire structure (such as the ones depicted in Figure 2) can be produced. The importance of such structures is that the magnetic character of Co can be used to our advantage as a new feature of transport in this system with the spin playing a significant role. The field of spintronics is a very active research area as well as a very important application topic since spintronic devices are now used in recording Magnetoresistance Random Access Memory (MRAM) for high density hard drives.[25] We believe that the use of magnetic atoms in nanostructures such as the system studied here can be a way of introducing spin dependent features into nanosystems.

Simulations of Au nanowires were able to follow the evolution of a thick wire under stress into a one-dimensional wire of five atoms connected to Au tips.[26] These wires were used to study many structural properties up to their rupture. The role of impurities in NWs led to many interesting results. One was the explanation of the large Au−Au bond distances observed in experiments[27] that led to the study of the effect of light impurities, which are today believed to be responsible for the observation of such large distances.[28] Another was the study of oxygen which showed that this impurity can help to make linear atomic chains (LACs) larger than those in pure Au NWs,[29] a fact that was experimentally observed.[30]

Here we propose a new structure, namely, a Au nanowire with a Co magnetic impurity as a new system in which novel and interesting spin effects can be observed and that can be used to make spintronic devices. We have used a Au metallic nanowire obtained in a previous molecular dynamics simulation,[26] with a one-atom constriction, and substituted this Au atom by a Co atom and relaxed its structure in order to study the structural, electronic, and transport behavior of this new nanowire. We show that if judicially chosen, this system exhibits quite striking new features such as enhanced spin conductance and a large spin polarization. We believe this construction mimics what can be done experimentally with the techniques mentioned above.

2. Methods

Electronic and structural properties of the NWs were performed with spin-polarized total energy Density Functional Theory (DFT)[31,32] calculations within the PBE-GGA approximation[33] with norm conserved pseudopotentials.[34] The calculations used the SIESTA code[35] with a DZ basis set with a confining energy shift of 0.002 Ry and a cutoff of 400 Ry for the grid integration. The system was elongated in steps of 0.5 Å. For each length the atomic positions were relaxed until the forces on all atoms were smaller than 0.03 eV/Å. Periodic boundary conditions in all directions were employed, with a supercell approximation with a lateral and upper separation of 20 Å to avoid the interaction between the images. Brillouin zone sampling of $1 \times 1 \times 2$ k-points was used.

The transport properties of the present system were studied using a combination of DFT and the nonequilibrium Green's function (NEGF) method.[38–42] The DFT was implemented with norm conserving pseudopotentials within the localized basis code SIESTA. The transport calculations were performed using the

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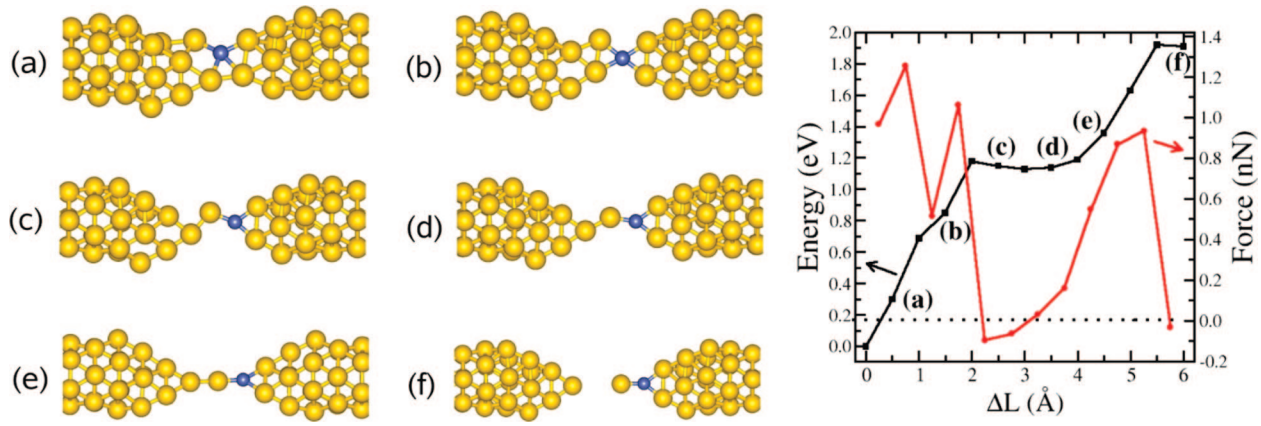

Figure 2. Left panel: Evolution of geometries for six selected structures of an Au NW with one Co atom, with increasing size up to its rupture. Right panel: Total energies (eV) and forces (nN) for all structures studied. Labels (a) to (f) refer to the structures presented in the left panel.

TRANSAMPA code[42] which is based on nonequilibrium Green's functions and DFT [NEGF-DFT]. The central quantity in TRANSAMPA as well as in other NEGF-DFT implementations is the Green function for the scattering region (S) given by:

$$G = \left(E^{+}S_S - H_S - \sum\nolimits_L(E) - \sum\nolimits_R(E)\right)^{-1} \quad (1)$$

where the self-energies $\Sigma_L(E)$ and $\Sigma_R(E)$ incorporate the effect of coupling between the electrodes and the scattering region, H_S is the Hamiltonian of S, and S_S is the overlap matrix. The scattering region S is schematically presented in Figure 1.

The NEGF-DFT is based on a mean-field description for the electronic structure at the scattering region. It is known to provide reliable results for metallic point contacts in the strong coupling regime between the leads and the scattering region, when the conductance is high,[43] which is the present case. However, as the Kondo effect has been observed[44] in STM experiments of Co atoms adsorbed in Au(111), it might be possible that such an effect could be observed in the present situation as well. Even though the present formalism cannot address this issue, one of our main goals which is to show the strong change in conductance as a function of the local symmetry will not be affected by the inclusion of strong local correlations, since it will not change the existence or nonexistence of the s−d coupling. Finally, it should be mentioned that even though scattering by phonons has been shown to play an important role in certain experimental situations,[20,45] at very low temperatures and low bias voltages, which is the situation we are considering in the present work, vibrations can be ignored since the electrons will traverse across the wire without dissipation.[45]

3. Results and Discussion

The Au nanowire with a one Co atom constriction is stable, and the relaxed structures obtained are shown in Figure 2. As is well-known Au is not magnetic, and for atomically thin Au nanowires the conductance is quantized with one quanta of conductance. The substitution of Au by Co as the neck atom that separates the two sides of the Au nanowire brings novelties to the behavior of the system. Co is an atom that has a partially occupied d-shell, and the first question that comes to mind is what is its influence to the otherwise nonmagnetic Au nanowire?

Such a NW with one Co impurity atom in the neck region was studied for different elongations caused by external stress. Figure 2 (left panel) shows the structure of the NW for six selected stages of the evolution until rupture. The initial structure is depicted in Figure 2a after relaxing the forces, and the reconstructed configuration presents two parallel chains, one formed solely by Au atoms and the other by gold atoms connected with the Co, thus forming two channels. Upon stretching, it evolved to the structure shown in Figure 2b where one Co atom connects the two tips. This new structure occurred due to the rearrangements of the atoms, which is reflected in the energy and mostly in the force, which presents large oscillations, as can be seen in Figure 2 (right panel). The next rearrangement corresponds to breaking of a bond, forming in this way an atomically thin chain (Figure 2c) with a zigzag configuration. Note that at this stage the force becomes negative, meaning that the structure is compressed. The evolution of the structure with three atoms in the neck, two Au atoms and one Co atom, occurs solely by the stretching of these three atoms, whereas the other distances in the tips remain with essentially the same bond lengths. The distance between the two tip atoms increases as the zigzag form opens up to produce a linear chain (Figure 2d−e). Finally, upon further stretching, the wire breaks at a Au−Au bond. Figure 2 (right panel) shows the total energies and forces during the evolution of the NW. At the early stages of the process major atomic rearrangements occur, which is evident from the oscillation of the force. The last three structures (from structure (d) to (f)) have an almost linear force increase and a parabolic energy curve characteristic of stretching of the zigzag chain, similar to the behavior of a spring, until the breaking that occurs at structure (f) with a force of approximately 1.0 nN. It is worthwhile to note that this rupture force is smaller than the observed forces[36,37] necessary to break a pure Au nanowire, which is on the order of 1.5 nN. This indicates that the presence of the Co atom is somehow making its neighboring Au−Au bond weaker than that in pure nanowires.

One of the most important properties of NWs, besides being the thinnest possible wires, is their conductance, since they have been used as electric nanocontacts. It is well-known that the conductance of a Au linear chain is approximately $1G_0$, the quantum of conductance ($G_0 = 2e^2/h$), the two spin channels giving the same degenerate value.[17] This corresponds to a featureless transmittance around E_F, the Fermi energy of the system. The inclusion of a magnetic impurity such as Co into this NW causes an interesting behavior with spin dependent features.

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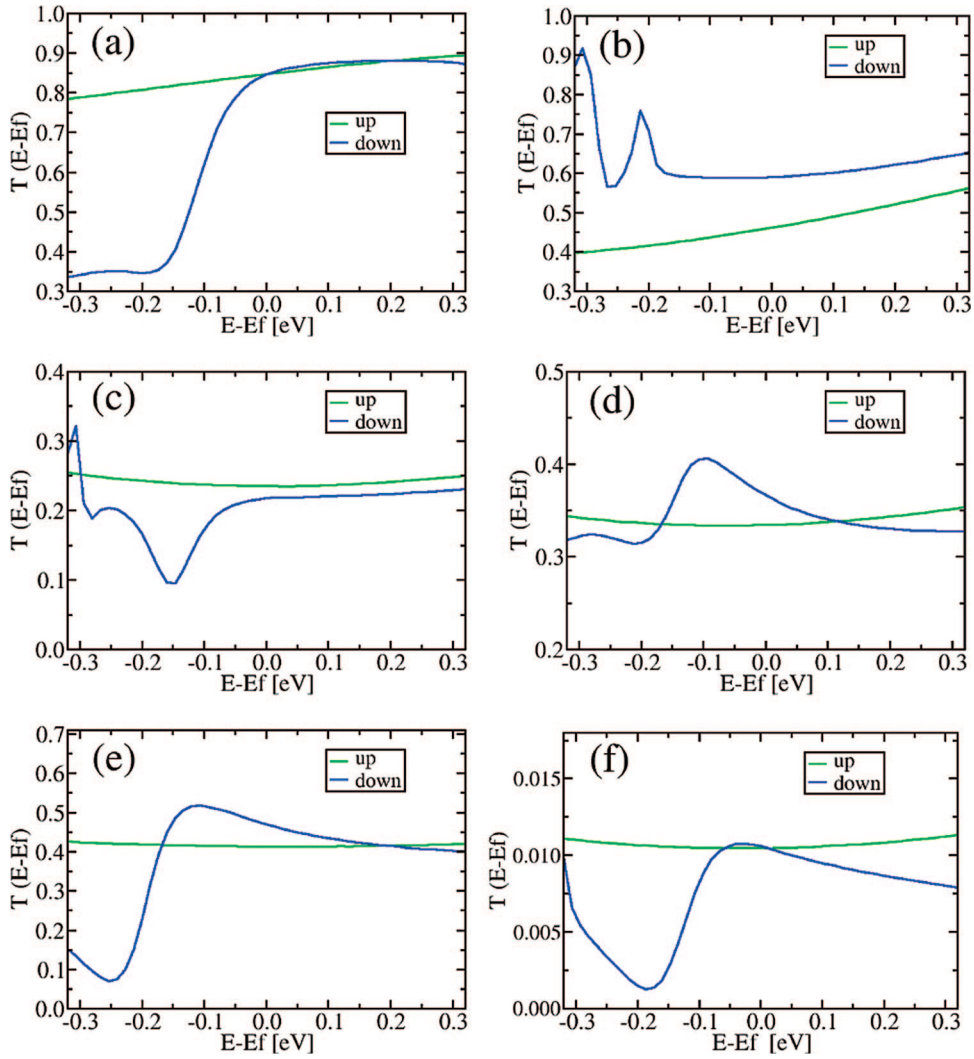

Figure 3. Transmittances (in units of $G_0 = 2e^2/h$) for the six structures displayed in Figure 2. All figures show T_{up} (green) and T_{down} (blue).

For all configurations the up channel transmittance is very much structureless in the energy region presented, around 0.35 eV of the Fermi level. An analysis of the projected density of states (PDOS) (see Figure 4) shows that this is a result of the absence of Co d-orbitals in this energy window. Thus, the transmittance has solely an s-character from both the Au and Co atoms. In the structure shown in Figure 3a the value of the transmittance is close to $1G_0$ for the up spin, indicative of two open channels which are associated with the thicker constriction. As a one-atom constriction is formed (Figure 3b), there is a decrease to a value closer to $0.5G_0$, as expected. With the formation of the zigzag configuration, there is an increase of the scattering due to the local geometry, and the transmittance becomes reduced. However, as the wire is stretched and the neck becomes linear, the transmittance slowly increases toward $0.5G_0$. For the down channel, as there are Co d-states in the energy window studied, the transmittance presents a lot of structures, which are a result of the interference between the s- and d-channels. One characteristic of this interference is the appearance of Fano-like resonances in the transmittance, a result of the competition between the delocalized s-like states and the more localized Co d-states. Structure (c), which has the zigzag chain, starts to show more clearly this feature of a Fano-like resonance. This resonance becomes enhanced as the NW is stretched, as can be seen in the transmittance of structure (d), and is then clearly present in structure (e). Further pulling breaks the NW. Note that in configuration (f) the transmittance scale is approximately 2 orders of magnitude smaller than that in the other structures.

Figure 3 presents the transmittance for the two spin channels T_{up} (up means majority spins) and T_{down} (down means minority spins), in units of G_0 for the six structures of Figure 2. This mixing between the s- and d-channels can be understood in terms of the local symmetry in the neck. The structure composed by the linear chain and the atoms that connect it to the leads have a local C_{2v} symmetry (see Figure 4). Within this symmetry group the s-orbitals of the Au atoms in the linear chain generate A_1 irreducible representations (IRs), whereas the s-orbitals in the four Au atoms that connect the chain to the leads generate A_1 and B_2 IRs. The Co s-orbital also generates an A_1 IR, and its d-orbitals generate A_1, A_2, B_1, and B_2 IRs. Thus, the Co s- and d-orbitals can mix with the Au s-orbitals, and the scattering states present interference effects.

This can be clearly seen in the PDOS for the s- and d-orbitals of the Au and Co atoms presented in Figure 4. There is a clear contribution coming from all these states in the energy window where the Fano-like resonance is present, with a lot of structures

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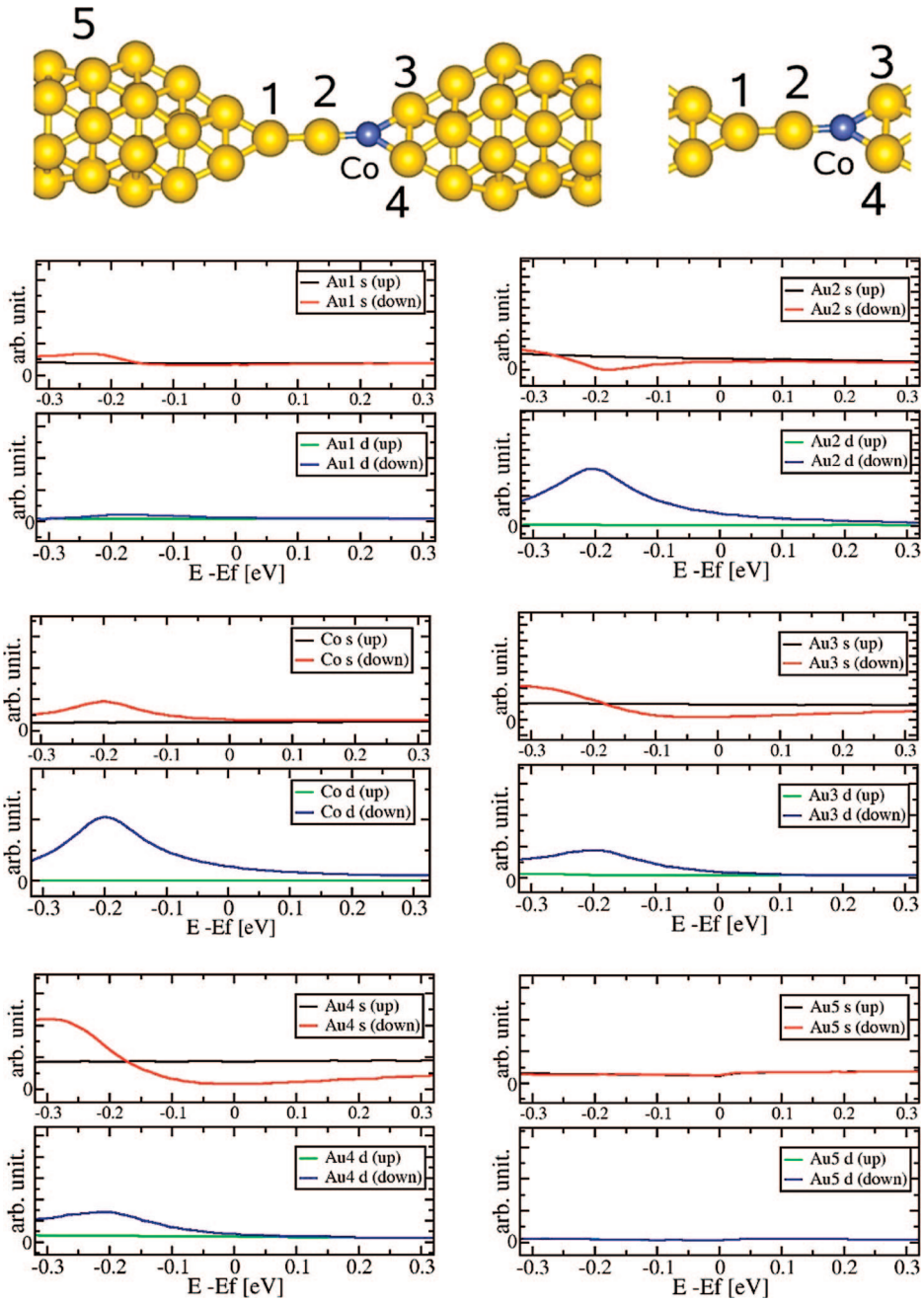

Figure 4. Upper panel: The structure (e) from Figure 2 is presented with a few selected atoms numbered. The inset on the right shows the neck and the atoms that connect it to the leads with a local C_{2v} symmetry. Lower panel: The projected densities of states (PDOS) for the selected atoms numbered in the upper panel. The PDOS were calculated using the Green′s function for the open system[46] (all the PDOS except the Co d-orbitals are multiplied by 10).

in the PDOS, indicating the relative phase changes. These structures in the PDOS are only present in the down spin channel, where the Co d-orbitals are present. Note that, in the up spin channel, as already mentioned, the PDOS is very much featureless, indicating simply an s-state contribution in the whole energy window.

Due to the asymmetric character of the scattering between the up and down channels, it is expected that there will be a nonzero charge transport spin polarization $\xi = (T_{up} - T_{down})/(T_{up} + T_{down})$. Focusing on the structure (e) where the Fano-like resonance is more pronounced, we calculate ζ to be equal to 0.07 at the Fermi level. This value is not larger because at the Fermi level the up and down transmittances are not very different, as can be seen in Figure 3e. However, we expect that as the energy is varied along the Fano resonance the polarization will show significant changes and the system could be possibly used as a spin filter.

In order obtain better insight in the transmittance and the role of Co and the local symmetry, we studied also a related structure, very possible to occur in such an experiment; namely we exchange Au(2) in Figure 4 (upper panel) with the Co to form a symmetrical Au−Co−Au LAC as shown in Figure 5 (upper panel), which will be called from now on SCo-NW.

The transmittance for such a structure is depicted in Figure 6. As can be seen, the up spin transmittance is still featureless, with a value close to $0.5G_0$. The character of the transport in this channel is basically related to Au and Co s-states, as can be observed from the PDOS shown in Figure 5. The down

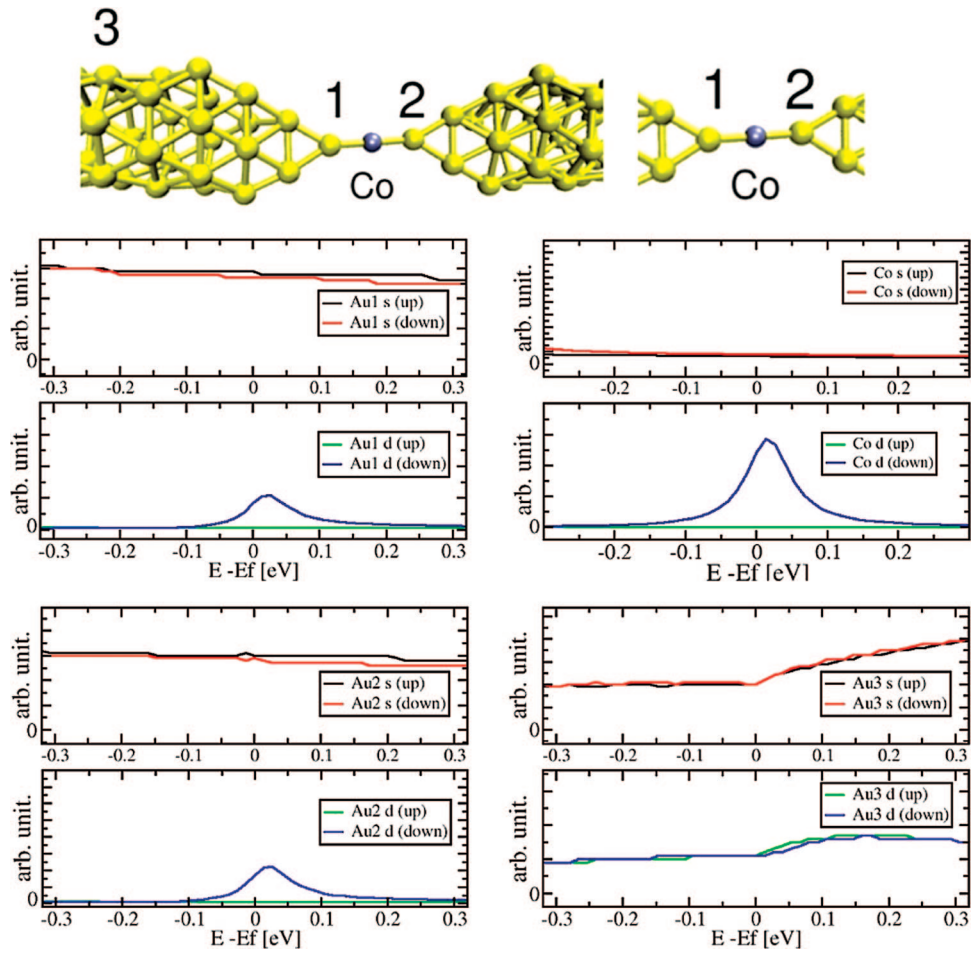

Figure 5. Upper panel: The symmetrical structure SCo-NW is presented with some selected atoms numbered. The inset on the right shows the neck and the atoms that connect it to the leads with a local D_{2h} symmetry. Lower panel: The projected densities of states (PDOS) for the selected atoms numbered in the upper panel. The PDOS were calculated using Green's function for the open system[46] (all the PDOS except the Co d-orbitals are multiplied by 10).

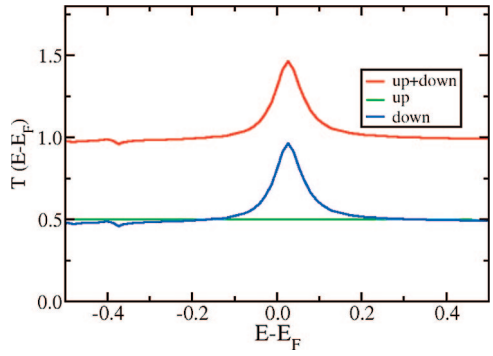

Figure 6. Transmittance for the symmetrically positioned Co atom structure shown in Figure 5. We present T_{up} (green), T_{down} (blue), and the total T (red).

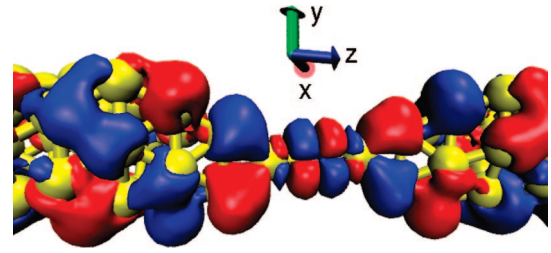

Figure 7. Kohn−Sham eigenvector associated with the d-state close to the Fermi level, for the SCo-NW. It clearly shows a d_{yz} character. Blue (red) indicates a positive (negative) value.

channel, on the other hand, has a clear peak close to the Fermi level, with a width on the order of 0.2 eV. Away from this peak the down channel transmittance is similar to the transmittance of the spin up states, indicating that it is also related to s-orbitals. Another distinct feature is the disappearance of the Fano-like resonance.

The explanation for this behavior is related to the local symmetry in the neck. The three atoms, Au(1), Co, and Au(2), plus the other four atoms that connect the linear chain to the leads (see inset in Figure 5) form a structure with a local D_{2h} symmetry group. Within this group, the Au(1) and Au(2) s-orbitals generate irreducible representations (IRs) with A_g and B_{1u} character, and the Co s-orbital belongs to the A_g IR. An analysis of the Co d-state close to the Fermi level, on the other hand, shows that it has a *yz* character (see Figure 7) and thus belongs to the B_{3g} IR. Therefore, the approximate local symmetry decouples the s- and d-channels around the Fermi level, destroying in this way the interference between these states, which is necessary for the presence of the Fano-like resonance. As a result, close to the Fermi level we simply have the sum of the contributions of the different channels, which are mostly s-dominated and d-dominated. In fact, the presence of this Co d-orbital close to the Fermi level brings a contribution of the Au d-states, which now contribute to the transmittance

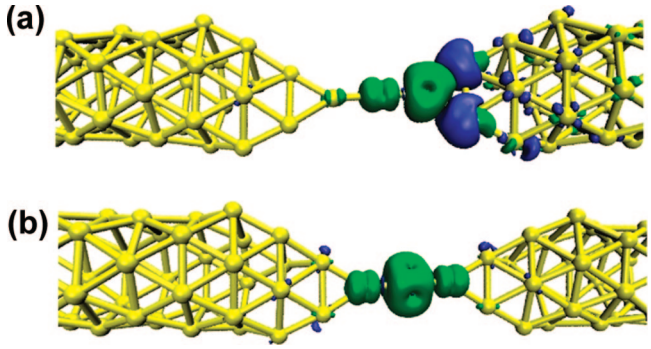

Figure 8. Local difference between the charge density for the up and down spins, $\rho_{up}-\rho_{down}$, for (a) the structure shown in Figure 1e and (b) SCo-NW. Green indicates spin up, whereas blue indicates spin down.

as well. This is the reason the total transmittance becomes larger than $1G_0$, which would be the upper limit if only s-states participated in the transport. Therefore, we have a situation where the local symmetry can dramatically change the transport properties, generating either Fano-like resonances or simply a peak related to the simple sum of transmittances where a great spin enhanced conductance can be produced. The value of the spin conductance anisotropy, $\xi = 0.23$, is now much larger than the value for the asymmetric structure (e) discussed previously.

All these transport features are connected to the net nonzero magnetization that is caused by the presence of the Co about. This magnetization is very localized in the Co and its nearest neighbors, as can be seen by the difference between the charge density for the up and down spins, which is proportional to the net spin magnetization, shown in Figure 8a for structure (e), where there is a positive magnetization at the Co tip and negative one for Au(3) and Au(4). The SCo-NW structure (Figure 8b) on the other hand has a magnetization restricted to the LAC, being positive for both the Co and its two Au neighbors.

4. Summary

In summary, we have shown that the insertion of a transition metal atom in a Au NW can result in strong spin dependent transport properties. In particular, the local symmetry of the nanowire can dramatically change these transport properties. When such symmetry permits the mixing between the wire s-orbitals with the transition metal d-states, there are interference effects that resemble Fano-like resonances. On the other hand, if this symmetry decouples such states, we simply have a sum of independent transmission channels. This opens up new vistas to the field of nanospintronics. With the present manipulation techniques, it is possible to design wires connected to systems with the appropriate local symmetry in such a way that spin anisotropy effects are enhanced. For example, connecting the wire discussed in the present work to magnetic leads can lead to a spin filter with the ultimate size limit, which can be used to explore spintronic devices at a new scale.

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