We calculate the conductances and the tunneling magnetoresistance (TMR) of double magnetic tunnel junctions, taking as a model example junctions composed of Fe/ZnSe/Fe/ZnSe/Fe (001). The calculations are done as a function of the gate voltage applied to the in-between Fe layer slab. We find that the application of a gate voltage to the in-between Fe slab strongly affects the junctions’ TMR due to the tuning or untuning of conductance resonances mediated by quantum well states. The gate voltage allows a significant enhancement of the TMR, in a more controllable way than by changing the thickness of the in-between Fe slab. This effect may be useful in the design of future spintronic devices based on the TMR effect, requiring large and controllable TMR values.

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Double-barrier magnetic tunnel junctions (DBMTJs), in which metallic layers are inserted in between the semiconducting region of single-barrier MTJs (SBMTJs), are nowadays gaining an increasing interest due to their potential advantages over SBMTJs in spintronic devices based on the tunneling magnetoresistance effect (TMR)\(^1\). Although the idea of using double-barrier junctions goes back to the work of Zhang *et al* a decade ago\(^2\), these hybrid systems could be epitaxially grown only quite recently.

For example, T. Nozaki *et al* \(^3\) have recently measured the TMR of fully epitaxial Fe/MgO (001) DBMTJs and found larger TMR and \(V_{1/2}\) values as compared to identically-grown single-barrier junctions (\(V_{1/2}\) is the bias voltage at which the TMR drops to half its value at infinitesimal bias voltage). Z. M. Zeng *et al* \(^4\) have also measured large TMR and \(V_{1/2}\) values in Co-Fe-B/Al-oxide double junctions. Other experimental works along the same lines that confirm these features include Refs. 5 and 6.

Besides their importance for spintronics applications, DBMTJs are interesting hybrid systems on their own since they exhibit richer transport phenomena than conventional tunnel junctions, that are currently under intense investigation. Among these phenomena we can mention the spin-dependent resonant tunneling due to quantum well states (QWS) inside the in-between metallic slab (IBS)\(^7,8\) and the spin-filter effect\(^9−11\). Both effects have been theoretically investigated using realistic electronic structure models only recently\(^9,10,12\). The picture that emerges from these theoretical and experimental studies is that double-barrier junctions have three major properties unavailable in single-barrier ones. First, the TMR values of DBMTJs are, in general, significantly larger than those of similarly prepared SBMTJs. Second, the dependence of the TMR on bias voltage is considerably smaller in DBMTJs than in SBMTJs. And third, the differential conductance of DBMTJs shows well defined peaks as a function of bias voltage\(^8,13\). The first two features can be qualitatively understood in terms of the spin-filter effect\(^9\). The origin of this effect is the spin-dependent potential introduced by the in-between magnetic layers, which quenches the conductance for the antiparallel magnetic configuration of the junction. The third property is related to resonant tunneling through quantum well states that form in the in-between metallic slab\(^6,9,12,13\).

From the above, it is clear that the investigation of the spin-dependent transport properties of this kind of junctions is worthwhile. In this work we consider, as a model example, Fe/ZnSe (001) double-barrier junctions, and calculate their coherent conductances and TMR. We focus on the dependence of the conductances and of the TMR on the gate voltage applied to the in-between Fe slab. This is an aspect that has not been, to our knowledge, studied so far. Starting with the pioneering calculations of Zhang *et al* \(^2\), the main reason for using double-barrier junctions has
been to enhance the TMR by controlling the thickness of the in-between metallic slab. It was theoretically shown by several authors\textsuperscript{7} that the TMR of DBMTJs depends on this thickness, essentially due to the tuning or untuning of conductance resonances mediated by quantum well states (see, for example, the recent experimental work of Niizeki \textit{et al} \textsuperscript{8}). Although it is nowadays possible to control the differential conductance by varying the thickness of the in-between metallic slab with sub-monolayer precision, in this work we propose to control the TMR values of DBMTJs in another way, namely, by a gate voltage applied to the in-between slab. We analyze this possibility within a simple yet realistic model. We note that gate-control has been studied in other systems as well, such as carbon nanotubes and quantum dots (see, for instance, Ref. 14 and references therein).

Our main conclusion is that the gate voltage is an important degree of freedom to enhance the TMR value of DBMTJs, which may be experimentally rather easily available. It allows the tuning and untuning of the various conductance resonances arising in double-barrier junctions (thus enhancing or quenching the TMR), in a similar way the thickness of the IBS does, but much more easily from the practical standpoint. Furthermore, the very large and controllable TMR values obtained in gate-biased double-barrier junctions are not attainable using conventional single-barrier junctions.

\section{Systems Under Study and Calculation Methods}

Our DBMTJs consist of $m$ layers of BCC Fe (001) inserted in between $2n$ layers of zinc-blende ZnSe, so that the Fe midlayers are sandwiched by $n$ identical ZnSe layers at each side, the whole multilayer (which we will call active region or AR) being sandwiched by two semi-infinite BCC Fe (001) electrodes. We fix $n =$2, which represents 1.13 nm of ZnSe at each side of the in-between Fe slab (IBS), and consider $m =$2, 3, 4, 6, representing 0.574, 0.861, 1.148, 1.722 nm of in-between iron. The junctions are periodic in the $x$-$y$ plane, being $z$ the transport direction. We note that the junctions are fully epitaxial and that interface interdiffusion is not taken into account.

In the parallel configuration ($P$), the magnetizations of all the magnetic regions (electrodes and in-between Fe layers) are parallel to each other. In the antiparallel configuration ($AP$), the electrodes’ magnetization remain parallel to each other but the Fe midlayer’s magnetization is antiparallel to them. It is important to note that, since the coercive fields of the electrodes and of the midlayer are different (due to their different thicknesses), these magnetic configurations are experimentally attainable, as has been shown in recent years.

The electronic structure of the junctions is modeled by a Slater-Koster\textsuperscript{15} second nearest neighbors \textit{spd} tight-binding Hamiltonian fitted to \textit{ab initio} band structure calculations for bulk Fe and bulk ZnSe\textsuperscript{16}. To calculate the mixed
hoppings between the Fe and the (Zn,Se) atoms in the junctions, we use Shiba’s rules and Andersen’s scaling law\textsuperscript{17}.

The Fe $d$ bands are spin split by $\mu J_{dd}$, where $\mu=2.2 \mu_B$ is the experimental magnetic moment of bulk Fe and $J_{dd}=1.16$ eV is the exchange integral between the Fe $d$ orbitals ($\mu_B$ is Bohr’s magneton). With these values for $\mu$ and $J_{dd}$, the bulk Fe $d$ bands’ spin splitting is very well reproduced. We have also checked that the electrodes’ and the spacer’s band structures compare very well to FP-LAPW calculations performed with the \textit{Wien2k} code\textsuperscript{18}. The complex band structure of ZnSe, that determines which evanescent states inside the semiconducting region are able to couple to Bloch states inside the electrodes, is also very well reproduced as compared to \textit{ab initio} calculations\textsuperscript{19,20}. The conductances and the TMR of Fe/ZnSe simple junctions, as a function of the energy of the incident electrons and of the spacer’s thickness, are also in very good agreement with the first principles results of MacLaren et al\textsuperscript{20}. In our DBMTJs, the midlayer Fe $d$ bands’ splitting is the same as the one corresponding to bulk Fe. This is a rather good approximation since several experimental works\textsuperscript{21} have shown that the magnetic moment of Fe slabs approaches that of bulk Fe even for very thin layers. When forming the junctions, the ZnSe tight-binding on-site energies are rigidly shifted to make the Fe Fermi level fall 1.1 eV below its conduction band minimum, as indicated in photoemission experiments performed on Fe/ZnSe thin films\textsuperscript{22}. The gate voltage applied to the in-between Fe is simulated by a rigid shift of the on-site energies of the Hamiltonian describing the isolated in-between Fe slab. We note that Lee et al\textsuperscript{23} have been able to fabricate double junctions in which the in-between metallic slab could be gate-biased, so that the DBMTJs that we study here are, in principle, experimentally possible.

The ballistic conductances $\Gamma$ are obtained from Landauer’s formalism expressed in terms of Green’s functions\textsuperscript{24}. The Green’s function describing the dynamics of an electron inside the active region $(\text{ZnSe}(n)/\text{Fe}(m)/\text{ZnSe}(n))$ is given by

$$G^\sigma_S = \left[ \mathbf{1} E_F - H_S^\sigma - \Sigma_L^\sigma - \Sigma_R^\sigma - \Sigma_g^\sigma \right]^{-1}$$

where $\mathbf{1}$ stands for the unit matrix, $E_F$ is the Fermi energy of the system, and $H_S^\sigma$ is the active region’s Hamiltonian ($\sigma$ corresponds to the majority or minority spin channels). We note that $H_S^\sigma$ depends on the applied gate voltage $V_g$, since the on-site energies of the Fe atoms of the IBS are rigidly shifted by $V_g$. In Eq. (1), $\Sigma_{L/R}^\sigma$ are the self-energies describing the interaction of the AR with the left ($L$) and right ($R$) electrodes, while $\Sigma_g^\sigma$ are the self-energies due to the gate electrode contacted to the in-between Fe slab. The self-energies due to the iron electrodes are given by

$$\Sigma_L^\sigma = H_{LS}^\dagger g_L^\sigma H_{LS} \quad \text{and} \quad \Sigma_R^\sigma = H_{RS}^\dagger g_R^\sigma H_{RS}$$

where $H_{LS}$ and $H_{RS}$ are the tight-binding couplings of the active region with the electrodes, and $g_{L/R}^\sigma$ are the surface
Green’s functions for each electrode. The surface Green’s functions are calculated using a semi-analytical method and are exact within our tight-binding approximation. The self-energies \( \Sigma^g_\sigma \) are taken as complex parameters (wave vector and gate-bias independent), where the real and imaginary parts represent the shifting and the broadening (finite life-time) of the energy levels of the IBS due to their coupling to the gate electrode. In order to simulate a paramagnetic gate electrode whose band structure near \( E_F \) along the \((001)\) direction is similar to that of majority (maj.) Fe electrons but not to that of minority (min.) Fe ones (for example, gold), we fix the imaginary parts of \( \Sigma^{maj./min.}_g \) at the constant (energy-independent) values of \(-0.05\) eV and \(-0.01\) eV, respectively, corresponding to lifetimes \( \frac{\hbar}{-2\text{Im}[\Sigma^{maj./min.}_g]} \) of \(6.58\) fs and \(32.9\) fs. With such values we are assuming that the IBS majority electrons can leak to the gate electrode more easily than the minority ones, because the latter are more confined due to the band structure mismatch between the IBS minority bands and the gate electrode’s bands. The real parts of \( \Sigma^{maj./min.}_g \) are calculated as the principal part of the Hilbert transforms of \(-2\text{Im}[\Sigma^{maj./min.}_g]\), in order to ensure that \( \Sigma^g_\sigma \) are causal (retarded). At \( E_F \), the real parts of \( \Sigma^{maj./min.}_g \) are equal to \(0.12\) eV and \(0.015\) eV, respectively.

The transmission probabilities for the transition from the left to the right electrodes, \( T^\sigma \), are given by

\[
T^\sigma(k_{//}, E_F) = Tr \left[ \Delta^\sigma_L G^\sigma_S \Delta^\sigma_R G^{\sigma\dagger}_S \right]
\]

(3)

where \( \Delta^{\sigma}_{L/R} = i(\Sigma^\sigma_{L/R} - \Sigma^{\sigma\dagger}_{L/R}) \) are the hybridization functions of the active region with the \((L,R)\) electrodes. \( T^\sigma \) gives the probability that an electron coming from the left electrode reaches the right electrode. Processes in which an electron enters and leaves the gate electrode are not taken into account. That is to say, we calculate the conductance due to electrons that tunnel directly from one electrode to the other, through the active region whose electronic structure is renormalized by the presence of the gate electrode. The conductances are then given by \( \Gamma^\sigma(E_F) = \frac{e^2}{\hbar N_{k_{//}}} \sum_{k_{//}} T^\sigma(k_{//}, E_F) \), where \( N_{k_{//}} \) is the total number of wave vectors parallel to the interface that we consider in our calculations. The tunneling magnetoresistance coefficient is defined as \( \text{TMR} = 100 \times (\Gamma_P - \Gamma_{AP})/\Gamma_{AP} \) (optimistic definition), where \( \Gamma_P \) and \( \Gamma_{AP} \) are the conductances in the \( P \) and in the \( AP \) magnetic configurations, respectively.

By calculating \( \Gamma \) using different numbers of parallel-to-the-interface wavevectors \( k_{//} = k_x \hat{x} + k_y \hat{y} \) (recall that the junction is periodic in the \( x-y \) plane), we find that a mesh of 5000 \( k_{//} \) is enough to reach convergence. More details on the method used to calculate the conductances can be found in Ref. 10 (see also Ref. 25).

In this work, we restrict ourselves to zero temperature, to infinitesimal bias voltage (applied to the Fe electrodes) and to the coherent regime. We assume that the electron’s \( k_{//} \) and spin are conserved during tunneling, since the junctions are fully epitaxial and the Fe midlayer is thin (<2 nm) and ordered.
In Figs. 1-4, we show the conductances (upper panels) in the parallel and antiparallel configurations of double-barrier junctions with \( n = 2 \) layers (1.13 nm) and \( m = 2, 3, 4 \) and 6 layers (0.574, 0.861, 1.148 and 1.722 nm), respectively, together with the corresponding TMR values (lower panels), as a function of the applied gate voltage. The first thing to note from the upper panels of Figs. 1-4 is the appearance of sharp conductance peaks at certain values of the gate voltage. These peaks occur for both magnetic configurations \( P \) and \( AP \), and are a signature of resonant tunneling through polarized quantum well states inside the in-between Fe slab. Essentially, the evanescent states inside the ZnSe spacers (coupled to Bloch states inside the electrodes) can couple to quantum well states confined in the in-between Fe slab, thus producing transmission resonances. It is clearly seen that it is possible to sweep the quantum well states energy spectrum by sweeping the gate voltage. That is to say, by changing the gate voltage what we are doing is to move the quantum well states in energy. As already mentioned, something similar occurs when changing the thickness of the in-between Fe slab\(^7\). The QWS-mediated resonant tunneling phenomenon is displayed by all the DBMTJs that we considered. It is particularly clear in those DBMTJs with \( m = 3 \) and 6 layers, where sharp \( P \) and \( AP \) conductance peaks, respectively, are observed.

These conductance resonances have an enormous impact on the TMR, as it can be seen from the lower panels of Figs. 1-4. The TMR values of the DBMTJs that we consider are to be compared to the corresponding one for the single-barrier junction with \( n = 2 \) layers (1.13 nm), equal to 25 \%. It is seen that, even at \( V_g = 0 \), the TMR of DBMTJs is larger than that of the corresponding SBMTJ. It is also seen that the TMR of DBMTJs can reach, under resonant conditions, extremely large values. Considering gate voltage values close to zero, the gain in TMR obtained by applying a gate voltage is by a factor of 5, 100, 5, 3, for the \( m = 2, 3, 4, 6 \) DBMTJs, respectively. The TMR enhancement is particularly large for the DBMTJ with \( m = 3 \) layers, in which the TMR goes from 460 \% at zero gate (which is 20 times larger than the TMR of the \( n = 2 \) SBMTJ) to 47000 \% at -20 mV (which is almost 2000 times larger than the TMR of the SBMTJ). A large TMR increase also occurs in the double junction with \( m = 4 \) layers, where the TMR goes from 230 \% to 1000 \% by applying a gate voltage of 10 mV. The main conclusion from this analysis is that the TMR of double-barrier Fe/ZnSe junctions depends very strongly on the applied gate voltage, and that it can reach extremely large values not possible in single-barrier junctions. That is to say, the TMR of DBMTJs is, in general, significantly larger than that of SBMTJs, and it can be further enhanced by gate-biasing the double junctions.

Another very interesting feature to note is the occurrence of very large negative TMR values (in the optimistic
definition, the minimum TMR value is -100%). For example, the DBMTJs with \( m=2 \) layers (Fig. 1) has a very sharp AP conductance peak at a gate of -60 mV, which produces a TMR value very close to -100 %. The same happens for the \( m=6 \) DBMTJ (Fig. 4), at gate voltages equal to -40 mV and 120 mV. This switching of the TMR values from positive to negative and vice versa, in conjunction with the large TMR enhancements that we obtain as compared to the TMR of SBMTJs and of DBMTJs at zero gate voltage, may find a use in future spintronic devices requiring large and/or variable TMR values. With respect to this, we should mention that such large TMR values, both positive and negative, are not so far away from what can nowadays be experimentally attained. For example, A. Iovan and coworkers\(^6\) have very recently obtained TMR values as high as \( 10^4 \) % in Fe/MgO double-barrier junctions, the origin of which is resonant tunneling through spin-polarized Fe QWSs. Another possible application of gate-biased DBMTJs, making use of the very large TMR values attainable with these systems, is as magnetic field sensors based on the TMR effect\(^{26}\). One of the key parameters in these devices is the sensitivity of the TMR values on the applied magnetic field, and an increase in the TMR results in an increase in sensitivity. We have shown in this work that a viable way to obtain extremely large values of the TMR is to use gate-biased double-barrier magnetic tunnel junctions. It is expected that, if the value of the gate voltage is properly chosen so as to produce a large TMR value, the magnetic field sensitivity of the DBMTJ will greatly surpass the current sensitivity values attainable in single-barrier junctions\(^{26}\).

Although our calculations are not self-consistent (i.e. we do not take into account charge transfer effects at the junctions’ interfaces) and are performed at infinitesimal bias voltage, we believe that they still capture the essential point of this phenomenon. That is, the tuning or untuning of conductance resonances due to the shifting of quantum well states, and their impact on the tunneling magnetoresistance of double-barrier junctions. We think that the application of a gate voltage to the in-between metallic layers of a double junction is an issue that deserves further theoretical and experimental investigation. Control of the TMR by a gate voltage is better suited to applications than the fine tuning of the in-between metallic thickness, and may result in new functionalities for spintronics applications. Furthermore, this property is not restricted to Fe/ZnSe (001) DBMTJs, since the appearance of spin-polarized quantum well states in thin magnetic slabs sandwiched by insulating spacers is a rather general phenomenon\(^{6−9,12,13}\).

**IV. SUMMARY**

Taking as a model example junctions composed of Fe/ZnSe (001), we have calculated the coherent, zero-bias conductance and the tunneling magnetoresistance of double-barrier tunnel junctions, as a function of the gate voltage applied to the in-between Fe slab and of its thickness. The electronic structure of the junctions and their transport
properties were realistically calculated. We found that the tunneling magnetoresistance of double-barrier junctions is strongly dependent on the applied gate voltage, essentially due to the tuning or untuning of conductance peaks produced by resonant tunneling through quantum well states. The tunneling magnetoresistance can be tuned to extremely large values by sweeping the gate voltage. This feature is displayed by all the DBMTJs that we considered. The calculated TMR values of the gate-biased double junctions greatly surpass those attainable in single-barrier junctions, as well as those of double junctions at zero gate voltage. The most important qualitative conclusion is that the tunneling magnetoresistance can be dramatically enhanced by applying small gate voltages, which is more easily accessible than controlling the in-between slab’s thickness. Furthermore, it is possible to obtain large and negative TMR values as well. Since the complex band structures of ZnSe (001) and of MgO (001) are very similar to each other, we believe that these features should also be observed in Fe/MgO (001) double-barrier junctions as well. These findings may be useful in the design of spintronic devices relying on the tunneling magnetoresistance effect, and in consequence further theoretical and experimental investigation is desirable. For example, it would be very interesting to study the influence of the gate voltage on the dependence of the tunneling magnetoresistance on bias voltage, which is a critical aspect for applications.

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FIG. 1: Conductances (upper panel) and TMR (lower panel) of a double-barrier junction with $n=2$ (1.13 nm) and $m=2$ (0.574 nm), as a function of the applied gate voltage.

FIG. 2: Conductances (upper panel) and TMR (lower panel) of a double-barrier junction with $n=2$ (1.13 nm) and $m=3$ (0.861 nm), as a function of the applied gate voltage. The TMR peak at $V_g=-20$ mV has been reduced by a factor of 10 in order to fit in the graph.

FIG. 3: Conductances (upper panel) and TMR (lower panel) of a double-barrier junction with $n=2$ (1.13 nm) and $m=4$ (1.148 nm), as a function of the applied gate voltage.
FIG. 4: Conductances (upper panel) and TMR (lower panel) of a double-barrier junction with $n=2$ (1.13 nm) and $m=6$ (1.722 nm), as a function of the applied gate voltage.