Spin-filtering efficiency of ferrimagnetic spinels CoFe$_2$O$_4$ and NiFe$_2$O$_4$

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We assess the potential of the ferrimagnetic spinel ferrites CoFe$_2$O$_4$ and NiFe$_2$O$_4$ to act as spin filtering barriers in magnetic tunnel junctions. Our study is based on the electronic structure calculated by means of first-principles density functional theory within different approximations for the exchange correlation energy. We show that, in agreement with previous calculations, the densities of states suggest a lower tunneling barrier for minority spin electrons, and thus a negative spin-filter effect. However, a more detailed analysis based on the complex band-structure reveals that both signs for the spin-filtering efficiency are possible, depending on the band alignment between the electrode and the barrier materials and depending on the specific wave-function symmetry of the relevant bands within the electrode.

I. INTRODUCTION

The ability to generate and detect spin-polarized currents is a central requirement for any practical spintronics device. A promising approach to achieve this goal is to use tunnel junctions containing ferro- or ferrimagnetic barrier materials, thus presenting different tunneling probabilities for majority (spin-up, $\uparrow$) and minority (spin-down, $\downarrow$) electrons. Efficient spin-filtering has been demonstrated for ferromagnetic insulators such as EuS$^6$, EuO$^2$ and BiMnO$_2$. However the magnetic ordering temperatures of these magnets are rather low. Therefore the identification of suitable barrier materials that operate at room temperature or above is of great interest.

Spinel ferrites are insulating ferrimagnets with high Curie temperatures ($T_C$ = 790 K for CoFe$_2$O$_4$ and 865 K for NiFe$_2$O$_4$)$^2$ and therefore are promising candidates for efficient room temperature spin-filtering. A measure of the ability of a material or a device to select a particular spin direction is the spin-filtering efficiency, $P_{sf}$, which is defined as

$$P_{sf} = \frac{I^{\uparrow} - I^{\downarrow}}{I^{\uparrow} + I^{\downarrow}},$$

where $I^\sigma$ is the spin-$\sigma$ component of the current, which is assumed to be carried by the two spin species in parallel. Recent experiments on ferrimagnetic spinels appear promising, as a spin-filtering efficiency of $+22\%$ has been measured for NiFe$_2$O$_4$ at low temperatures.$^2$ The measured positive sign of $P_{sf}$ is in apparent contradiction with results of band-structure calculations, demonstrating that the bottom of the conduction band is lower for spin-down electrons than for spin-up,$^2$ which would lead to a lower tunneling barrier for minority spin electrons. It was suggested that this apparent discrepancy could be due to effects related to the wave-function symmetry of the tunneling states.$^2$ Furthermore, for CoFe$_2$O$_4$ both positive and negative $P_{sf}$ have been reported in junctions made of different electrode materials and where $P_{sf}$ was measured with different experimental techniques. The reported values of $P_{sf}$ range from $-44\%$ to $+26\%$.$^7,12$ Due to these large variations in experimental results (with both signs occurring for the spin-filtering efficiency) there is a need to provide a reference for future experimental studies and to allow further optimization of the corresponding devices.

So far, theoretical predictions for the spin-filter effect in CoFe$_2$O$_4$ and NiFe$_2$O$_4$ are almost exclusively based on density of states (DOS) calculations within a self-interaction corrected (SIC) local density approximation (LSDA).$^2$ The spin-splitting of the conduction band minimum (CBM) in these calculations suggests a lower tunnel barrier for minority spin electrons and thus a negative sign for the spin-filtering efficiency. However, it is well known that in many cases this simple density of states argument can be misleading, and the tunnel probability can be strongly dependent on the specific wave-function symmetry.$^{13}$ The implications of this were first noticed in a Fe/MgO/Fe heterostructure,$^{14,15}$ where symmetry-dependent tunneling results in half-metallic behaviour of the Fe/MgO(001) stack. Since then, the so-called complex band-structure, which determines the decay length of Bloch states with different wave-function symmetries inside an insulating barrier, has been used to account for many, otherwise unexplained, experimental results in spin-dependent tunnel junctions. Furthermore, it is of interest to compare the SIC-LSDA result of Ref.$^2$ to the electronic structure obtained by using alternative approaches such as LSDA+$U$, hybrid functionals, or other SIC approaches.

Here we present a detailed comparison of the electronic structure of CoFe$_2$O$_4$ and NiFe$_2$O$_4$ calculated within different approximations for the exchange-correlation potential. This allows us to identify features of the DOS that are fairly robust with respect to the specific choice of exchange-correlation potential and features that are very sensitive to this choice. In addition, we calculate the com-
plex band-structure for both materials within the atomic SIC method (ASIC)\textsuperscript{16,17}, which facilitates the identification of suitable electrode materials that can lead to high spin-filtering efficiency. We show that, for both CoFe$_2$O$_4$ and NiFe$_2$O$_4$ and the two transport directions [001] and [111], electrons tunnel with the highest probability at the center of the two-dimensional Brillouin zone in the plane orthogonal to the transport direction. Furthermore, depending on the exact alignment of the electrode Fermi level relative to the CBM of the barrier, the tunneling current may present either a predominant majority or a predominant minority contribution, i.e. $P_{d}$ may change sign depending on the level alignment.

The paper is organized as follows. After having briefly presented the computational method and the details of the crystallographic unit cell used for this study, we proceed to discuss the electronic structure of CoFe$_2$O$_4$ and NiFe$_2$O$_4$. In particular, we first discuss the DOS and real band-structures, and then move on to present the complex ones. The final section summarizes our main conclusions.

II. METHODS

We employ the VASP\textsuperscript{18} and SIESTA\textsuperscript{19} density functional theory (DFT) code packages for the calculation of DOS and real band-structures and the SMEAGOL code\textsuperscript{20,21} to calculate the complex band-structure. The VASP calculations have been performed by using the projector-augmented wave (PAW) method\textsuperscript{22}, with standard PAW potentials supplied with the VASP distribution, a 500 eV plane wave energy cutoff, and a $\Gamma$ centered 6×6×6 k-point mesh for the Brillouin zone sampling. We employ the generalized gradient approximation (GGA) according to the Perdew-Burke-Ernzerhof formulation\textsuperscript{23}, together with the Hubbard “+$U$” correction\textsuperscript{24} where $U = 3$ eV and $J = 0$ eV is applied to the d states of all transition metal cations, as well as the hybrid functional approach according to Heyd, Scuseria and Ernzerhof (HSE)\textsuperscript{25} using the standard choice for the fraction of Hartree-Fock exchange ($\alpha = 0.25$) and a reduced plane wave energy cutoff of 400 eV. When using the localised basis set code SIESTA, structural relaxations were performed using the GGA while the atomic self-interaction correction (ASIC) scheme was used to determine the electronic structure, including the complex band-structure. A 6×6×6 k-point Monkhorst-Pack mesh was used to converge the density matrix to a tolerance of $10^{-5}$ and a grid spacing equivalent to a plane-wave cutoff of 800 eV was used.

For most of our calculations we use the smallest possible unit cell (containing 2 formula units) to describe the inverse spinel structure. The corresponding distribution of cations on the spinel $B$ site lowers the space group symmetry from $Fd\bar{3}m$ to $Imma$\textsuperscript{26}. We also present some results obtained for a cation distribution with $P4_122$ symmetry, which requires a doubling of the unit cell to 4 formula units (the $k$-point sampling is then adjusted accordingly). We have previously shown that both $Imma$ and $P4_122$ are low energy configurations for the inverse spinel structure in CoFe$_2$O$_4$ and NiFe$_2$O$_4$, and that the specific cation arrangement has only a minor influence on the global electronic structure of these systems\textsuperscript{27}. We note that experimentally a disordered distribution of Fe$^{3+}$/Ni$^{2+}$ cations over the spinel $B$ site with effective cubic $Fd\bar{3}m$ symmetry, i.e. with no long-range cation order, is generally observed, even though recent indications for short range cation order in both NiFe$_2$O$_4$ bulk and thin film samples have been reported\textsuperscript{28,29}. For a more detailed comparison between the different cation configurations see Refs.\textsuperscript{27} and\textsuperscript{30}.

Structural relaxations have been performed at the GGA level, with all cations being fixed to their ideal cubic positions\textsuperscript{26}. The relaxed bulk lattice constants $a_{0}$ obtained by using VASP (SIESTA) are 8.366 Å (8.360 Å) and 8.346 Å (8.356 Å) for CoFe$_2$O$_4$ and NiFe$_2$O$_4$, respectively, and are in very good agreement with experimental data (see Ref.\textsuperscript{27} and references therein).

III. RESULTS AND DISCUSSION

A. Electronic structure

It has been previously shown that GGA leads to a half-metallic solution for CoFe$_2$O$_4$ and results in only a very small insulating gap in the case of NiFe$_2$O$_4$ (see e.g. Refs.\textsuperscript{26,31} and references therein). The DOS of CoFe$_2$O$_4$ and NiFe$_2$O$_4$ calculated by using a selection of beyond-GGA functionals are depicted in Fig.\textsuperscript{1}. It can be seen that all the studied exchange-correlation potentials lead to an insulating state for CoFe$_2$O$_4$ and an enhanced band gap for NiFe$_2$O$_4$. When compared to the GGA+$U$ band gaps, both the inclusion of Hartree-Fock exchange within the HSE calculation as well as the ASIC treatment leads to a large increase in the band gap values for both the Co and Ni based ferrite, with the largest band gaps obtained for HSE (see Table I). We also note that our results are consistent with recent HSE and LSDA+$U$ calculations for NiFe$_2$O$_4$\textsuperscript{26}.

| | CoFe$_2$O$_4$ | NiFe$_2$O$_4$ |
|---|---|---|
| $E_g$ | $\Delta$CBM | $E_g$ | $\Delta$CBM |
| GGA+$U$ | 0.52 | 0.92 | 0.83 | 0.86 |
| HSE | 1.60 | 1.09 | 2.32 | 1.00 |
| ASIC | 1.08 | 1.00 | 2.07 | 0.46 |

TABLE I. Band gap ($E_g$) and spin-splitting of the CBM ($\Delta$CBM) for CoFe$_2$O$_4$ and NiFe$_2$O$_4$ calculated with different exchange-correlation functionals. All values are in eV.
FIG. 1. (Color online) Total and projected DOS per formula unit for CoFe$_2$O$_4$ (left panels) and NiFe$_2$O$_4$ (right panels) calculated with different exchange-correlation potentials (from left to right: GGA+U, HSE and ASIC). The $t_{2g}$ and $e_g$ states of Fe, Co, and Ni on the $O_h$ sites and the $e$ and $t_2$ states of Fe on the $T_d$ sites are shown as black (blue) and dark grey (red) lines, respectively. The shaded grey area in all panels depicts the total DOS. Minority spin projections are shown using negative values. The zero energy is set to the middle of the band gap.

$p$ valence bands. Interestingly, for CoFe$_2$O$_4$ the valence band maximum in ASIC is made up of the majority spin Co $e_g$ states, whereas for both GGA+U and HSE the corresponding minority spin $t_{2g}$ states are slightly higher in energy. We also note that the difference in the calculated GGA+U band gap of CoFe$_2$O$_4$ (NiFe$_2$O$_4$) compared to the previously obtained values of 0.9 eV (0.97 eV) for the $Imma$ structure_, and 1.24 eV (1.26 eV) for the $P4_122$ structure, is due to the fact that in the present work all calculations are performed at the GGA volume, whereas the calculations in Refs. 26 and 27 have been performed at the larger GGA+U optimized volume. In addition to the expected dependence on the exchange correlation potential, our results thus indicate a strong volume sensitivity in particular of the calculated CoFe$_2$O$_4$ band gap. Experimental estimates for the band gaps of spinel ferrites are sparse and vary over a broad range comprised between 0.11 eV and 1.5 eV for CoFe$_2$O$_4$ and between 0.3 eV and 3.7 eV for NiFe$_2$O$_4$. A recent optical absorption study of NiFe$_2$O$_4$ suggests an indirect gap of 1.6 eV in the minority spin channel which thus represents an upper bound for the corresponding fundamental band gap.

In all cases, and for both CoFe$_2$O$_4$ and NiFe$_2$O$_4$, the CBM is lower in energy for the spin-down states than for spin-up ones, in agreement with the SIC-LSDA calculations of Ref. [6]. In the case of CoFe$_2$O$_4$, all the three approaches used in our work predict a spin-splitting of the CBM (ΔCBM in Table I) of around 1 eV. For NiFe$_2$O$_4$ however, GGA+U and HSE yield a ΔCBM of around 0.9-1.0 eV, while ASIC gives a somewhat smaller splitting of only 0.46 eV. In all the cases, the obtained spin-splittings of the CBM are smaller than those reported in Ref. 6.1.28 eV (1.21 eV) for CoFe$_2$O$_4$ (NiFe$_2$O$_4$). We note, however, that even smaller values, namely of 0.47 eV for both CoFe$_2$O$_4$ and NiFe$_2$O$_4$, have been obtained in previous GGA+U calculations at the relaxed GGA+U volume. Recent experiments estimate the spin-splitting of the CBM in the tens of meV range for CoFe$_2$O$_4$-containing junctions.

In order to shed further light on the nature of the bands around the gap, the calculated GGA+U and ASIC band structures for both CoFe$_2$O$_4$ and NiFe$_2$O$_4$ are shown in Fig. 2. Apart from the larger band gaps obtained by the ASIC approach, it can be seen that the relative energies of the minority and majority spin bands in the upper valence band region for CoFe$_2$O$_4$ differ between GGA+U and ASIC. This is consistent with our previous discussion of the DOS. For the calculation that is performed with GGA+U, the top of the valence band is formed by a minority spin band with maximum at the X point, i.e. the minority spin band gap is indirect. In contrast
a direct gap with mixed spin character at $\Gamma$ is obtained by ASIC. Since, as we will show in the following, the tunneling probabilities are dominated by states around the $\Gamma$ point, we do not expect that this qualitative difference between the two exchange-correlation functionals will critically affect the transport properties.

Based on our analysis of the DOS and the band-structure in the vicinity the gap, we can conclude that despite some differences, all computational methods consistently predict a lower tunnel barrier for the minority spin electrons and therefore a negative spin-filtering efficiency for both CoFe$_2$O$_4$ and NiFe$_2$O$_4$. However, as shown in Fe/MgO/Fe tunnel junctions in the case of high quality epitaxial interfaces between the electrodes and the barrier material such DOS considerations are only of limited value for the description of actual transport properties. Instead, the specific symmetry of the decaying wave-functions inside the barrier has to be considered. This can be achieved through calculation of the complex band-structure.

**B. Complex band structure**

The complex band-structure along a particular crystalline direction is calculated with the DFT non-equilibrium Green’s function code smeagol. The complex band-structure is nothing but the solution of the secular band equation extended to imaginary wave-vectors. Let us assume that the transport direction of a given tunnel junction is along the $z$ direction and that the material composing the barrier has a particular crystalline axis aligned along that direction. For any given $k$-vector in the transverse $x$-$y$ plane, $k_\parallel = (k_x, k_y)$, and for any energy, $E$, the band equation \( E(k_x, k_y, k_z) \) can be solved for $k_z$ if one admits imaginary solutions $k_z = q + i\kappa$. This means that the wave-function of an electron approaching the tunneling barrier with transverse wave-vector $k_\parallel$ exponentially decays into the barrier along the $z$ direction over a length-scale given by $1/\kappa$. Clearly such decay rate depends on the transverse $k$-vector and the energy, i.e. $\kappa = \kappa(k_x, k_y; E)$. Here we consider the situation of electron transport along both the [001] and [111] directions of the cubic spinel structure.

In Fig. 2 we plot the minimal value of $\kappa$ as a function of $k_x$ and $k_y$ (calculated on a 100×100 grid) at different energies within the gap. We include data for both CoFe$_2$O$_4$ and NiFe$_2$O$_4$ considering both transport directions for the Imma configuration, and we also present data for the P4$_1$22 configuration and transport along the [001] direction. The crucial result emerging from Fig. 2 is that in all cases $\kappa$ is smallest at the $\Gamma$ point of the two-dimensional Brillouin zone corresponding to the x-y plane. This means that, due to the exponential dependence of the wave-function on $\kappa$, electron tunneling away from the $\Gamma$ point will contribute very little to the transport. As such, in the analysis that will follow, we will only consider transport through the $\Gamma$-point. We note that $\Gamma$-point filtering is a highly desirable property for both tunnel junctions and spin injection. As has been shown for the Fe/MgO barrier, as the thickness of the MgO layer increases so does the selectivity of the $\Gamma$-point. This in turn increases the tunneling magneto-resistance (TMR). Although the $\Gamma$-point filtering is not strictly necessary for a large TMR, it significantly reduces the importance of the material choice for the electrodes.

Having established that the transport predominantly occurs at the $\Gamma$-point, further insight can be gained by exploring the energy dependence of $\kappa(0, 0; E)$. In particular it is important to establish the spin and orbital symmetry of the complex bands corresponding to the smallest value of $\kappa(0, 0; E)$ for each energy, since incident waves with that particular symmetry will dominate the tunneling current. In Fig. 2 we present the complex band-structures of CoFe$_2$O$_4$ and NiFe$_2$O$_4$, calculated along the [001] and [111] directions at the $\Gamma$-point in the transverse 2D Brillouin zone for the Imma configuration. One can easily recognize that, for both CoFe$_2$O$_4$ and NiFe$_2$O$_4$, the main features which we discuss in the following are similar for the two different transport directions. We note that the transport calculation along [111] requires a larger unit cell, in order to obtain lattice vectors that are either perpendicular or parallel to the transport direction, which leads to a larger number of complex bands.
(a) *Imma*-CoFe$_2$O$_4$, transport along [001]

(b) *Imma*-CoFe$_2$O$_4$, transport along [111]

(c) *P4$_122$*-CoFe$_2$O$_4$, transport along [001]

(d) *Imma*-NiFe$_2$O$_4$, transport along [001]

(e) *Imma*-NiFe$_2$O$_4$, transport along [111]

(f) *P4$_122$*-NiFe$_2$O$_4$, transport along [001]

FIG. 3. Minimal value of $\kappa$ at different energies (indicated at the top left in each graph) within the gap for CoFe$_2$O$_4$ (a-c) and NiFe$_2$O$_4$ (d-f) along different transport directions, calculated within the ASIC approach. Zero energy corresponds to the middle of the band gap.

FIG. 4. The complex band-structure corresponding to $k_x = k_y = 0$ for NiFe$_2$O$_4$ (upper two panels) and CoFe$_2$O$_4$ (lower two panels) along [001] and [111], calculated within ASIC for the *Imma* ionic configuration. The up and down arrows indicate the spin-character of the lowest lying complex bands. The vertical dashed lines indicate the energies that were used for the $k_x$-$k_y$ plots in Fig. 3.

compared to the [001] case. In both materials the slowest decay rate close to the valence band maximum corresponds to electrons with majority spin character (in agreement with the real band-structure shown in Fig. 2). This remains the case for energies up to around 0.5 eV from the top of the valence band, although the decay rate increases quickly with energy. In contrast, the lowest decay rate for energies taken in the upper part of the band gap is dominated by states with minority spin symmetry. For NiFe$_2$O$_4$ this decay rate remains almost constant for a wide energy window of about 1.5 eV, whereas for CoFe$_2$O$_4$ the gap region is divided more symmetrically between the majority and minority spin-dominated regions. The smaller ASIC calculated band gap of CoFe$_2$O$_4$ compared to that of NiFe$_2$O$_4$ results in slightly slower decays within the gap region for both majority and minority spins.

In Fig. 4 we also present the complex band structure of CoFe$_2$O$_4$ and NiFe$_2$O$_4$ in the *P4$_122$* configuration.
FIG. 5. The complex band-structure corresponding to $k_x = k_y = 0$ for NiFe$_2$O$_4$ (upper panel) and CoFe$_2$O$_4$ (lower panel) along [001] for the $P4_{1}22$ configuration, calculated within ASIC. The up and down arrows indicate the spin-character for some of the lowest lying complex bands.

for transport along [001]. One can recognize the slightly larger band-gap compared to the $Imma$ configuration, but for NiFe$_2$O$_4$ the complex bands look very similar compared to the $Imma$ case. For CoFe$_2$O$_4$ one can see that the bands in the mid-gap region connect in a somewhat different way than in the $Imma$ configuration. However, the spin-characters of the lowest complex band in the upper and lower gap region remain unaffected by the different cation distribution, even though the energy range dominated by the minority spin complex bands is somewhat more extended in the $P4_{1}22$ case.

From the complex bands it becomes clear that positive as well as negative values for $P_{sf}$ are possible for both NiFe$_2$O$_4$ and CoFe$_2$O$_4$, depending on whether the Fermi level of the electrode lies in the upper or lower gap region of the spinel tunnel barrier, and on the availability of majority or minority spin carriers in the metal. If the Fermi level of the metallic electrode lies within $\sim 0.5$ eV from the top of the valence band, the slowest decay rate in both CoFe$_2$O$_4$ and NiFe$_2$O$_4$ will be for electrons with majority spin. In contrast, if the Fermi level of the electrode is more than $0.5$ eV above the valence band edge of the spinel barrier, then the slowest decaying state is in the minority spin channel. The exact position of the Fermi level of the metal depends on the band alignment between the two materials. Thus, the spin filter efficiency of the spinel ferrite barrier will depend strongly on the band alignment and eventually also on the orbital symmetry of the electrode states at the Fermi level. In addition, a good lattice match is of course required, otherwise translational symmetry is broken in the transverse plane and the complex band-structure argument breaks down. Here, the possibility to grow good quality films of CoFe$_2$O$_4$ and NiFe$_2$O$_4$ with either [001] or [111] orientation (see e.g. Refs. 32–34) opens up a wide range of possible electrode materials. In fact, high quality epitaxial junctions of CoFe$_2$O$_4$ or NiFe$_2$O$_4$ with various electrode materials, such as La$_2$/3Sr$_{1}$/3MnO$_3$, Au, Fe$_3$O$_4$, Nb-doped SrTiO$_3$, Pt, Co, Al, and SrRuO$_3$, have already been fabricated. 35–37

So far we have only discussed the spin character of the complex bands, whereas it is well known from the Fe/MgO/Fe system, that the orbital character of the relevant bands can also have a crucial influence on the tunneling properties. The determination of orbital character of the complex bands in the inverse spinel ferrites CoFe$_2$O$_4$ and NiFe$_2$O$_4$ is complicated by the different symmetries of the specific cation configurations used in the calculations. For example, the lowest lying state above the gap at $\Gamma$ in $Imma$-NiFe$_2$O$_4$, i.e. the one which connects to the complex band with minority spin character that has the smallest extinction coefficient over a rather large energy region within the gap, transforms according to the fully symmetric irreducible representation $A_g$ of the corresponding orthorhombic point group $mmm$. This means that, assuming an electrode with cubic bulk symmetry, this state can in principle couple to $\Delta_1$ and $\Delta_2$/$\Delta_2'$ bands for transport along the [001] direction (whether $\Delta_2$ or $\Delta_2'$ depends on how exactly the electrode is oriented with respect to the spinel structure), or to $\Delta_1$ and $\Delta_3$ for transport along the [111] direction. However, these considerations hold only for the case with $Imma$ symmetry and it is unclear how different cation arrangement, in particular a completely disordered cation distribution, would change these symmetry-based selection rules. Generally, the lower symmetry of the various cation arrangements leads to fewer symmetry restrictions regarding the possible coupling with electrode bands. Since a full symmetry analysis of all combinations that can possibly occur is beyond the scope of this paper, we restrict our analysis to the spin character of the decaying states within the barrier, which was discussed in the preceding paragraphs.

IV. SUMMARY AND CONCLUSIONS

In summary, we have calculated the electronic structure of both NiFe$_2$O$_4$ and CoFe$_2$O$_4$ using different approaches to evaluate the exchange-correlation potential. These include GGA, GGA+$U$, HSE and ASIC. We found that, while there are certain characteristic differences in the predicted band-structure, the densities of states of all beyond-GGA methods consistently suggest a lower tunnel barrier for minority spin electrons. Due to the well-known limitations of this simple density of states picture of tunneling, we have further analyzed the complex bands of the two materials at the ASIC level.

We have shown that the tunneling along the [001] and [111] directions is dominated by zone-center con-
tributions ($k_x = k_y = 0$), and that for both NiFe$_2$O$_4$ and CoFe$_2$O$_4$ the spin character of the slowest decaying state changes within the gap. Therefore, NiFe$_2$O$_4$ and CoFe$_2$O$_4$ are both capable of acting as either positive or negative spin filters, depending on the band alignment and wave-function symmetry of the electrodes. Given such a relatively sensitive dependence of the tunneling current on the position of the electrode Fermi level, we envision that gating may allow the spin filtering to be switched from positive to negative.

However, we also want to note that based on the complex band-structure of the barrier alone, it is not possible to make a definite prediction about the transport properties observed in a specific experiment. One may still encounter a situation where incident wave-functions with the desired symmetry, i.e. matching that of the smallest $\kappa(0, 0; E)$ inside the barrier, are not available within the electrodes, simply because of the corresponding real band-structures. Furthermore, it has been demonstrated recently for the case of an Fe-MgAl$_2$O$_4$-Fe tunnel junction, i.e. containing a non-magnetic spinel as barrier material, that the different unit cell sizes of the spinel barrier and the Fe electrodes can open up new transport channels due to “backfolding” of bands from the in-plane Brillouin zone boundary onto the Γ point. This leads to a relatively low tunnel magneto-resistance for the Fe-MgAl$_2$O$_4$-Fe junction, even though the corresponding complex and real band structures would indicate a highly symmetry-selective barrier. Therefore, in order to fully assess the spin-filter efficiency for a specific combination of electrode and barrier materials, a full transport calculation for the entire device needs to be performed. Nevertheless, the analysis of the complex band-structure provides a powerful interpretative tool and offers a good indication on what are the dominant contributions to the tunneling current. In the present case, it allows the rationalization of both signs of the spin-filter efficiency occurring in NiFe$_2$O$_4$ and CoFe$_2$O$_4$ tunnel junction, depending on the band alignment with the electrode.

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