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## Potential of AlP and GaN as barriers in magnetic tunnel junctions

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**AlP and GaN are wide band gap semiconductors used industrially in light emitting diodes. We investigate their potential as tunnel barriers in magnetic tunnel junctions, employing density functional theory and the non-equilibrium Green's function method for ground state and quantum transport calculations, respectively. We show that the valence band edges are dominated by  $p_z$  orbitals and the conduction band edges are dominated by  $s$  orbitals. Both materials filter Bloch states of  $\Delta_1$  symmetry at the  $\Gamma$ -point of the Brillouin zone. In the zero bias limit, we find for the Co/AlP/Co junction a high tunnel magnetoresistance of  $\sim 200\%$  at the Fermi energy and for the Co/GaN/Co junction a tunnel magnetoresistance of even  $\sim 300\%$  about 1.4 eV below the Fermi energy.**

where  $D_{\uparrow/\downarrow}$  is the majority/minority spin density of states at the Fermi energy ( $E_F$ ). Therefore, a TMR of  $\sim 60\text{--}70\%$  should be accessible in junctions based on transition metals irrespective of the electronic properties of the tunnel barrier, which disagrees with the experimental situation. In the early nineties of the last century, a TMR of  $\sim 20\%$  was established for amorphous  $\text{Al}_2\text{O}_3$  as tunnel barrier at room temperature.<sup>6,7</sup> Later, it was found that the tunnel current in many cases is not proportional to the density of states.<sup>8</sup> The major breakthrough, however, was the prediction in the early 2000s that in epitaxial junctions an arbitrarily large TMR is possible.<sup>9,10</sup> Here the transverse wave vector  $k_{\parallel}$  is conserved during the tunneling and the electron encounters different resistance based on the spin alignment of the electrodes and the symmetry of the wavefunction.

In the case of coherent transport the TMR depends on the tunnel currents  $I_P$  and  $I_{AP}$  under parallel (P) and antiparallel (AP) spin alignments of the electrodes as

$$\text{TMR} = (I_P - I_{AP})/I_{AP} \quad (2)$$

After a TMR of  $\sim 230\%$  was found at room temperature,<sup>11,12</sup> Fe/MgO/Fe junctions were adopted for applications such as spin-transfer torque devices,<sup>13,14</sup> microwave generators,<sup>15</sup> non-volatile full adders,<sup>16</sup> non-volatile field programming gate arrays,<sup>17</sup> non-volatile flip-flops,<sup>18–20</sup> static random access memories,<sup>21</sup> comparators,<sup>22</sup> neuromorphic computers,<sup>23–26</sup> magnetic read heads,<sup>27</sup> non-uniform clock generators,<sup>28</sup> sensors,<sup>29,30</sup> analog-to-digital converters,<sup>31–33</sup> not-and gates,<sup>34</sup> embedded memories,<sup>35</sup> radio-frequency spectrum optimizers,<sup>36</sup> and oscillators.<sup>37</sup>

While symmetry filtering is a general concept applicable to a variety of interfaces such as  $\text{Co}_2\text{MnSi}/\text{MgO}$ ,<sup>38</sup>  $\text{SrTiO}_3/\text{BaTiO}_3$ ,<sup>39</sup>  $\text{Cu}/\text{EuO}$ ,<sup>40</sup>  $\text{Co}/\text{h-BN}$ ,<sup>41</sup>  $\text{Fe}/\text{HfO}_2$ ,<sup>42</sup> and  $\text{Co}/\text{SiO}_2$ ,<sup>42</sup> only the FeCoB/MgO interface is currently used in main-stream applications. This is partially due to the possibility of B-assisted epitaxial growth of the Fe/MgO/Fe junction, which enables high transmission of spin-polarized current. The generation and detection of spin-polarized current are principal prerequisites for any spintronics device. While the Fe/MgO/Fe

## 1. Introduction

While the first evidence of anisotropic magnetoresistance was established by Lord Kelvin in Fe,<sup>1</sup> in the early seventies of the last century tunneling magnetoresistance (TMR) was reported for the Fe/Ge/Co junction at 4 K.<sup>2</sup> However, mainly the discovery of giant magnetoresistance<sup>3,4</sup> expedited the field of spintronics and now is one of its backbones. In giant magnetoresistance devices a non-magnetic metal, such as Cu or Pt, is sandwiched between ferromagnetic electrodes, offering two resistance states depending on the spin alignment of the electrodes. In TMR devices the non-magnetic metal is replaced with an insulator.<sup>5</sup> An electron tunneling through the barrier encounters different resistance depending on the Bloch state symmetry and spin alignment of the electrodes.

In the case of incoherent transport the TMR depends on the spin-polarizations  $P_{1/2} = (D_{\uparrow} - D_{\downarrow})/(D_{\uparrow} + D_{\downarrow})$  of the electrodes (1) and (2) as

$$\text{TMR} = 2P_1P_2/(1 - P_1P_2), \quad (1)$$

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junction plays a central role on this front, it suffers from disadvantages in fabrication, as the four-fold rotationally symmetric MgO must be grown on the six-fold rotationally symmetric face centered cubic [111] plane of the Ir–Mn/Co–Fe/Ru/Fe stack. Both Co and Ni provide the required six-fold rotation symmetry.<sup>43</sup> Moreover, the rather large Gilbert damping of the ferromagnets Fe and Co (ref. 44) impedes the magnetic quantum bit flipping by spin transfer torque in magnetoresistive random-access memories and the microwave generation by precession of the magnetic moment, for example.

Semiconductor junctions, on the other hand, offer new functionalities for optoelectronics and magnetic quantum bit devices to be potentially integrated with the current complementary metal–oxide semiconductor technology, bring memory elements close to logic elements, and help to realize spin-based displays.<sup>45</sup> In valleytronics the valley dependence of a spin-polarized current, mostly due to the broken inversion symmetry in crystal structures such as wurzite, is exploited.<sup>46</sup> It is therefore vital to explore new tunnel barrier materials to achieve junctions that can operate at or above room temperature with high TMR and provide high spin-polarized current. For this reason, we present here a detailed theoretical analysis of junctions based on the wurzite crystal structure using AlP or GaN as tunnel barrier and Co, Ni, or Fe as ferromagnetic electrodes. AlP and GaN are wide band gap semiconductors that are extensively used in the optoelectronics industry in light emitting diodes, whereas Co, Ni, and Fe are strong ferromagnets with high Curie temperatures. Analyzing such junctions has the potential to open new avenues in spintronics.

The paper is organized as follows: we first introduce our methodology and the technical details of our calculations. Then we discuss the real and complex band structures of the tunnel barriers and electrodes. Afterwards, we analyze the TMR and present our conclusions.

## II. Computational details

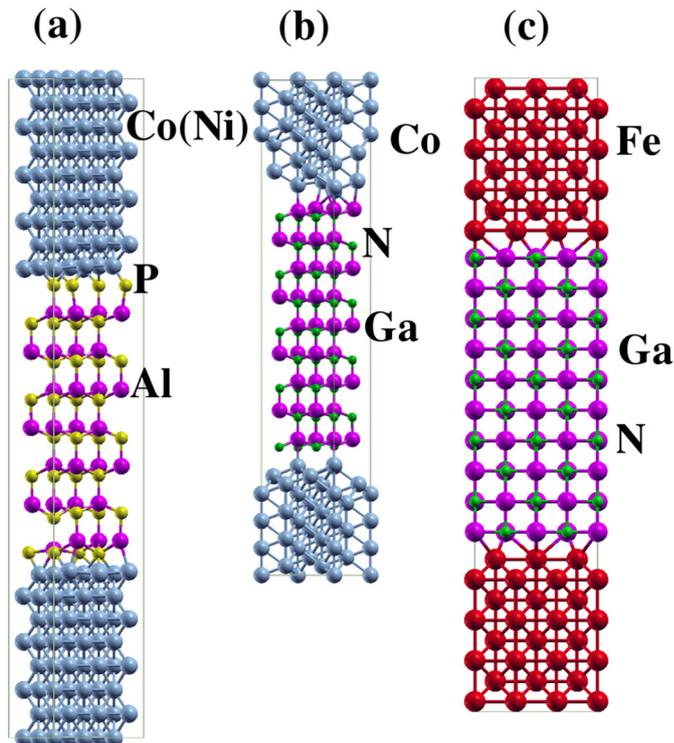
We employ Kohn–Sham density functional theory for performing ground state electronic structure calculations. The exchange–correlation potential is treated in the local density approximation as parameterized by Ceperley and Alder.<sup>47</sup> The Siesta engine is used with norm-conserving non-relativistic Troullier–Martins pseudopotentials<sup>48</sup> and a localized atomic-orbital basis set. The *s*, *p*, and *d* orbitals of Co, Ni, and Fe are expanded in a double- $\zeta$  basis set, while the *s* and *p* orbitals of Al, P, Ga, and N are expanded in a double- $\zeta$  plus polarization basis set. The band gaps of AlP and GaN are improved by the atomic self-interaction correction.<sup>49,50</sup> We use a grid spacing equivalent to a plane wave cutoff of 400 Ryd and a Monkhorst–Pack  $8 \times 8 \times 8$  *k*-mesh. The complex band structure along the *z*-direction is derived from the secular equation with  $k_{\parallel} = 0$ , *i.e.*, sampling is not required along this direction.

We study the

- Co[0001]/AlP[0001]/Co[0001],
- Ni[0001]/AlP[0001]/Ni[0001],

- Co[111]/GaN[0001]/Co[111], and
- Fe[001]/GaN[001]/Fe[001]

junctions seen in Fig. 1. The Co/AlP/Co and Ni/AlP/Ni junctions are constructed from hexagonal close packed (*hcp*) AlP with the in-plane lattice constant compressed by 2.8% from 3.86 Å (optimized value in the local density approximation) to 3.75 Å to achieve epitaxy between  $2 \times 2$  AlP[0001] and  $3 \times 3$  *hcp*-Co[0001] (lattice constant 2.50 Å (ref. 51)) or *hcp*-Ni[0001] (lattice constant 2.50 Å in the local density approximation). The Co/GaN/Co junction is constructed from wurzite GaN with the in-plane lattice constant stretched by 4.9% from 3.19 Å (ref. 52) to 3.34 Å to achieve epitaxy between  $2 \times 2$  GaN[0001] and  $3 \times 3$  body centered cubic (*bcc*) Co[111] with the in-plane lattice constant compressed by 4.5% from 2.86 Å (ref. 53) to 2.73 Å. The Fe/GaN/Fe junction is constructed from zinc blende GaN (lattice constant 4.50 Å (ref. 54)) by achieving epitaxy between  $2 \times 2$  GaN[001] and  $3 \times 3$  *bcc*-Fe[001] with the in-plane lattice constant stretched by 4.8% from 2.86 Å (ref. 53) to 3.00 Å. The thicknesses of the AlP[0001], GaN[0001], and GaN[001] tunnel barriers are chosen as 22.5, 16.1, and 24.8 Å, respectively (four unit cells). By structural relaxation using the conjugate gradient method, we reduce the forces acting on the atoms in the junctions to less than 0.01 eV Å<sup>-1</sup>. The junctions are asymmetric with broken inversion symmetry, which lifts the spin transmission degeneracy for AP spin alignment of the electrodes.



**Fig. 1** Structures of the (a) Co/AlP/Co and Ni/AlP/Ni, (b) Co/GaN/Co, and (c) Fe/GaN/Fe junctions. The junctions are asymmetric with broken inversion symmetry, resulting in different chemical environments at the two ends of the tunnel barrier.



For performing transport calculations, we employ the Smeagol engine,<sup>55–57</sup> which is interfaced with the Siesta engine and adopts the non-equilibrium Green's function method. In this formalism the left/right (L/R) electrode is described by a complex self-energy  $\Sigma_{L/R}^\sigma(E)$ , where  $\sigma = \uparrow$  or  $\downarrow$  is the spin and  $E$  is the energy. The effective Green's function of the central scattering region then is given by

$$G_C^\sigma(E) = \lim_{\eta \rightarrow 0} [E + i\eta - H_C^\sigma - \Sigma_L^\sigma(E) - \Sigma_R^\sigma(E)]^{-1}, \quad (3)$$

where  $H_C^\sigma$  is the Hamiltonian. The coupling matrix is

$$\Gamma_{L,R}^\sigma(E) = i(\Sigma_{L,R}^{\sigma+}(E) - \Sigma_{L,R}^{\sigma-}(E)), \quad (4)$$

where superscript  $+/-$  indicates the retarded/advanced part of the self-energy, and the transmission coefficient is given by

$$T^\sigma(E) = \text{Tr}[\Gamma_L^\sigma(E)G_C^{\sigma\dagger}(E)\Gamma_R^\sigma(E)G_C^\sigma(E)]. \quad (5)$$

As the junction is translationally invariant in the transverse plane, we can write:

$$T^\sigma(E) = \frac{1}{\Omega_{\text{BZ}}} \int_{\text{BZ}} d\mathbf{k}_\parallel T_{\mathbf{k}_\parallel}^\sigma(E), \quad (6)$$

where  $\Omega_{\text{BZ}}$  is the volume of the two-dimensional Brillouin zone (BZ),  $\mathbf{k}_\parallel = (k_x, k_y)$ , and  $T_{\mathbf{k}_\parallel}^\sigma(E)$  is the  $\mathbf{k}_\parallel$ -dependent transmission coefficient. From the transmission coefficients  $T_P(E)$  and  $T_{\text{AP}}(E)$  under P and AP spin alignments of the electrodes, we obtain

$$\text{TMR} = (T_P(E) - T_{\text{AP}}(E)) / T_{\text{AP}}(E), \quad (7)$$

where

$$T_{P/\text{AP}}(E) = T_{P/\text{AP}}^\uparrow(E) + T_{P/\text{AP}}^\downarrow(E). \quad (8)$$

The transport calculations are performed with a density matrix converged to a tolerance of  $10^{-4}$ .  $T^\sigma(E)$  is then calculated using a  $50 \times 50 \times 1$   $k$ -mesh. We notice no significant change in  $T^\sigma(E)$  or the TMR for a  $100 \times 100 \times 1$   $k$ -mesh.

### III. Results and discussion

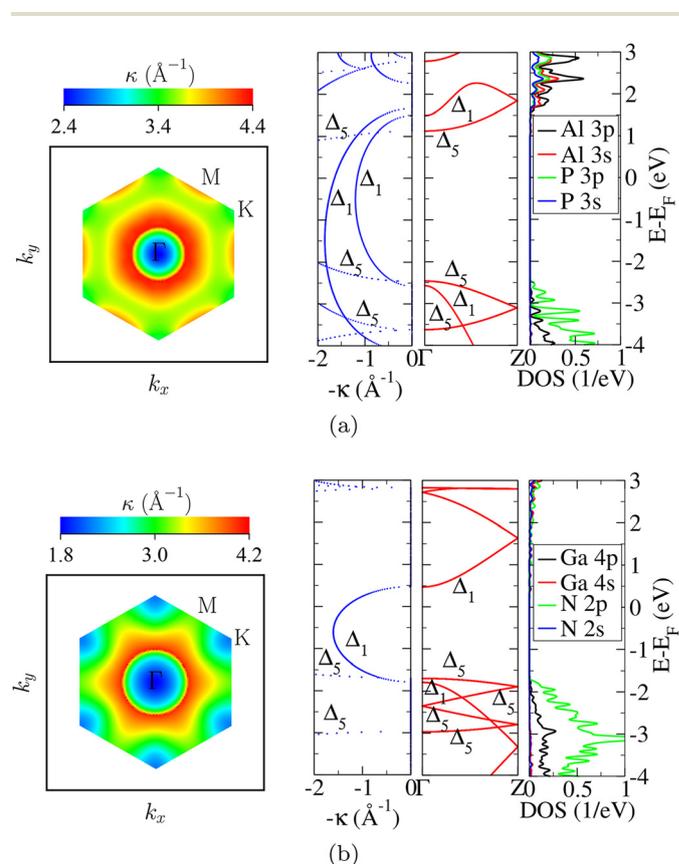
#### A. AIP and GaN as tunnel barriers

The band gaps of 1.5 eV (indirect) for AIP and 0.8 eV (direct) for GaN obtained in the local density approximation strongly underestimate the experimental values of 2.5 eV (ref. 58) and 3.3 eV,<sup>59</sup> respectively, while the atomic self-interaction correction improves them to 2.2 and 2.6 eV. These values are reduced to 1.5 and 2.0 eV, respectively, under the applied strains, while the band dispersions at the valence and conduction band edges remain similar (and are not critical in the tunneling regime) and the symmetries of the Bloch states are preserved. The symmetries of the Bloch states are also preserved for *bcc*-Fe and *bcc*-Co under the applied strains. The complex wave vector in the tunnel barrier is given by ( $k_z = ik$ ):

$$\kappa = \sqrt{2m(U - E)/\hbar^2 + \mathbf{k}_\parallel^2 - \langle \phi | \frac{\partial^2}{dx^2} + \frac{\partial^2}{dy^2} | \phi \rangle / \langle \phi | \phi \rangle}, \quad (9)$$

where  $U$  is the tunnel barrier height,  $\phi$  is the wavefunction, and the Laplacian term accounts for the transverse curvature effect of the wavefunction. As a function of the tunnel barrier thickness  $d$ , we expect a decay  $T(E, \mathbf{k}_\parallel) \sim T_0(E, \mathbf{k}_\parallel)e^{-2\kappa(E, \mathbf{k}_\parallel)d}$ , where  $T_0(E, \mathbf{k}_\parallel)$  depends on the atomic composition and nature of the interface (epitaxial or amorphous).

We plot  $\kappa(E_F, \mathbf{k}_\parallel)$  in Fig. 2 to establish the high transmission regions dominating the tunnel current. Minima at the  $\Gamma$ -point correspond to the situation that the tunneling electrons approach the barrier in normal direction, *i.e.*, the effective barrier thickness is minimal. While  $\Gamma$ -point driven transport is neither a necessary nor a sufficient condition for a high TMR, the typical parabolic energy dispersions around the  $\Gamma$ -point often result in  $\Delta_1$  symmetry of the Bloch states along the transport direction. Complying with this symmetry condition severely constrains the selection of ferromagnets. The decay of the evanescent states is similar in AIP and GaN due to the similar band gaps and electronic couplings, with the valence band edges dominated by  $p_z$  orbitals and the conduction band edges dominated by  $s$  orbitals. Note that the size of the band



**Fig. 2** Electronic structure analyses of (a) AIP and (b) GaN. The left panel shows a heat map of  $\kappa(E_F, \mathbf{k}_\parallel)$  in the BZ, reaching from the minimal to the maximal value. The right panels show the real (red) and complex (blue) band structures along the [0001] direction as well as partial densities of states.



gap affects the magnitude of  $\kappa(E_F, \mathbf{k}_{\parallel})$  but not the distribution in the BZ. Therefore, it affects the magnitude of  $T(E)$  but not the underlying physics.

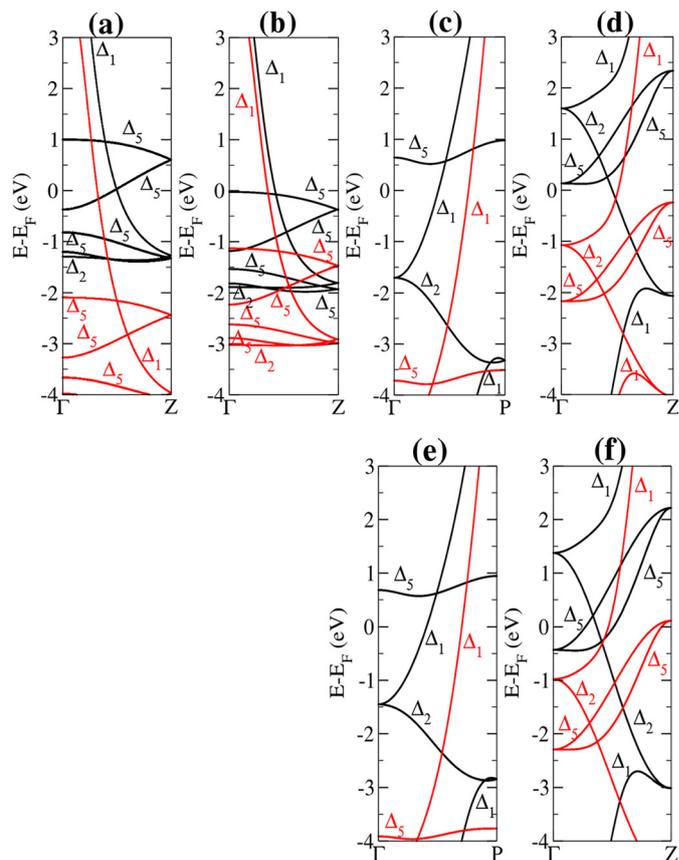
Next we analyze the real and complex band structures along the transport direction to relate them later with those of the electrodes. Generally, in epitaxial junctions the spin-flip and interband scatterings are minimal. As the same symmetry of the Bloch states is required to tunnel through the barrier, a strong coupling of the electrodes with the valence and conduction band edges of the semiconductor results in a high current. If only one spin channel of the ferromagnet is present at  $E_F$  then a highly spin-polarized current is expected. Note that our analysis of  $T(E)$  in terms of the electronic bands and their symmetry at the  $\Gamma$ -point is only qualitative, because the entire BZ contributes to  $T(E)$ . However, the main contribution is due to the region around the  $\Gamma$ -point, since there  $\kappa(E_F, \mathbf{k}_{\parallel})$  is minimal.

The symmetry of a Bloch state is assigned by analyzing its orbital composition after projecting it into the  $xy$ -plane (perpendicular to the transport direction). In particular,  $\Delta_1$  symmetry corresponds to  $s$ ,  $p_z$ , and  $d_{3z^2-r^2}$  orbitals with zero angular momentum in the transport direction,  $\Delta_5$  symmetry to  $p_x$ ,  $p_y$ ,  $d_{xz}$ , and  $d_{yz}$  orbitals,  $\Delta_2$  symmetry to  $d_{x^2-y^2}$  orbitals, and  $\Delta_2'$  symmetry to  $d_{xy}$  orbitals. The symmetries of the different bands at the  $\Gamma$ -point are shown in the real and complex band structures of AlP and GaN in Fig. 2. We find no ghost states in the complex band structures, which can appear for a non-orthogonal basis set.<sup>60</sup> Both semiconductors filter  $\Delta_1$  symmetry at the  $\Gamma$ -point. In the case of AlP, a valence band of  $\Delta_1$  symmetry with weak decay in the tunnel barrier connects to close to the conduction band edge. A valence band of  $\Delta_5$  symmetry connects directly to the conduction band edge, but, due to its strong decay, hardly contributes to  $T(E)$  unless  $E_F$  of the junction is pinned close to the valence band edge. In the case of GaN, a valence band of  $\Delta_1$  symmetry with weak decay connects to the conduction band edge.

## B. Ferromagnetic electrodes

We consider *hcp*-Co, *hcp*-Ni, *bcc*-Co, and *bcc*-Fe as ferromagnetic electrodes. To achieve a high TMR, the ferromagnet should have only one spin channel at  $E_F$  (behave as half-metal) with the symmetry of the wavefunction matching that of the tunnel barrier. Then the junction exhibits an exponential thickness dependence of the TMR. An example of this situation is the Fe/MgO/Fe junction, in which Fe supplies in the [001] transport direction majority spin  $\Delta_1$  Bloch states and both majority and minority spin  $\Delta_5$  Bloch states. MgO filters the  $\Delta_1$  symmetry at the  $\Gamma$ -point, resulting in an enormous TMR of  $\sim 10\,000\%$ .<sup>9,10</sup>

The real band structures of the four considered electrode materials are plotted in Fig. 3 along the transport directions. We find for both *hcp*-Co and *hcp*-Ni at  $E_F$  a majority spin band of  $\Delta_1$  symmetry and minority spin bands of  $\Delta_1$  and  $\Delta_5$  symmetries. For *bcc*-Co both majority and minority spin bands of  $\Delta_1$  symmetry are present at  $E_F$ , shifted in energy due to the exchange field. The different band dispersions (effective masses) will manifest in different contributions to  $T(E)$ . As the bands of  $\Delta_5$  symmetry show limited dispersions, the bands of  $\Delta_1$  and  $\Delta_2$



**Fig. 3** Real band structures of (a) *hcp*-Co, (b) *hcp*-Ni, (c) *bcc*-Co, and (d) *bcc*-Fe along the [0001], [0001], [111], and [001] directions, respectively. The majority spin bands are shown in red color and the minority spin bands are shown in black color. The Bloch state symmetry is indicated. Panels (e) and (f) show results analogous to panels (c) and (d), respectively, but without strain.

symmetries are expected to dominate  $T(E)$ . For *bcc*-Fe we find at  $E_F$  majority spin bands of  $\Delta_1$  symmetry. There are also both majority and minority spin bands of  $\Delta_5$  symmetry present at  $E_F$ , but they show limited dispersions. Due to the dispersive majority and minority spin bands of  $\Delta_2$  symmetry, however, it is expected that both spin channels are relevant for  $T(E)$ .

## C. Tunnel magnetoresistance

The momentum-dependence of the number of majority and minority spin transport channels at  $E_F$  is addressed in Fig. 4. For *hcp*-Co (six-fold rotation symmetry) we find an increased concentration of majority spin transport channels in a circular region around the  $\Gamma$ -point, while the minority spin transport channels are spread across the entire BZ. For *hcp*-Ni (six-fold rotation symmetry) both the majority and minority spin transport channels are concentrated in a ring around the  $\Gamma$ -point. For *bcc*-Co (six-fold rotation symmetry) the majority and minority spin transport channels are concentrated inside and outside a circular region around the  $\Gamma$ -point, respectively. Finally, for *bcc*-Fe (four-fold rotation symmetry) increased concentrations of both majority and minority spin transport channels appear along the symmetry axes.



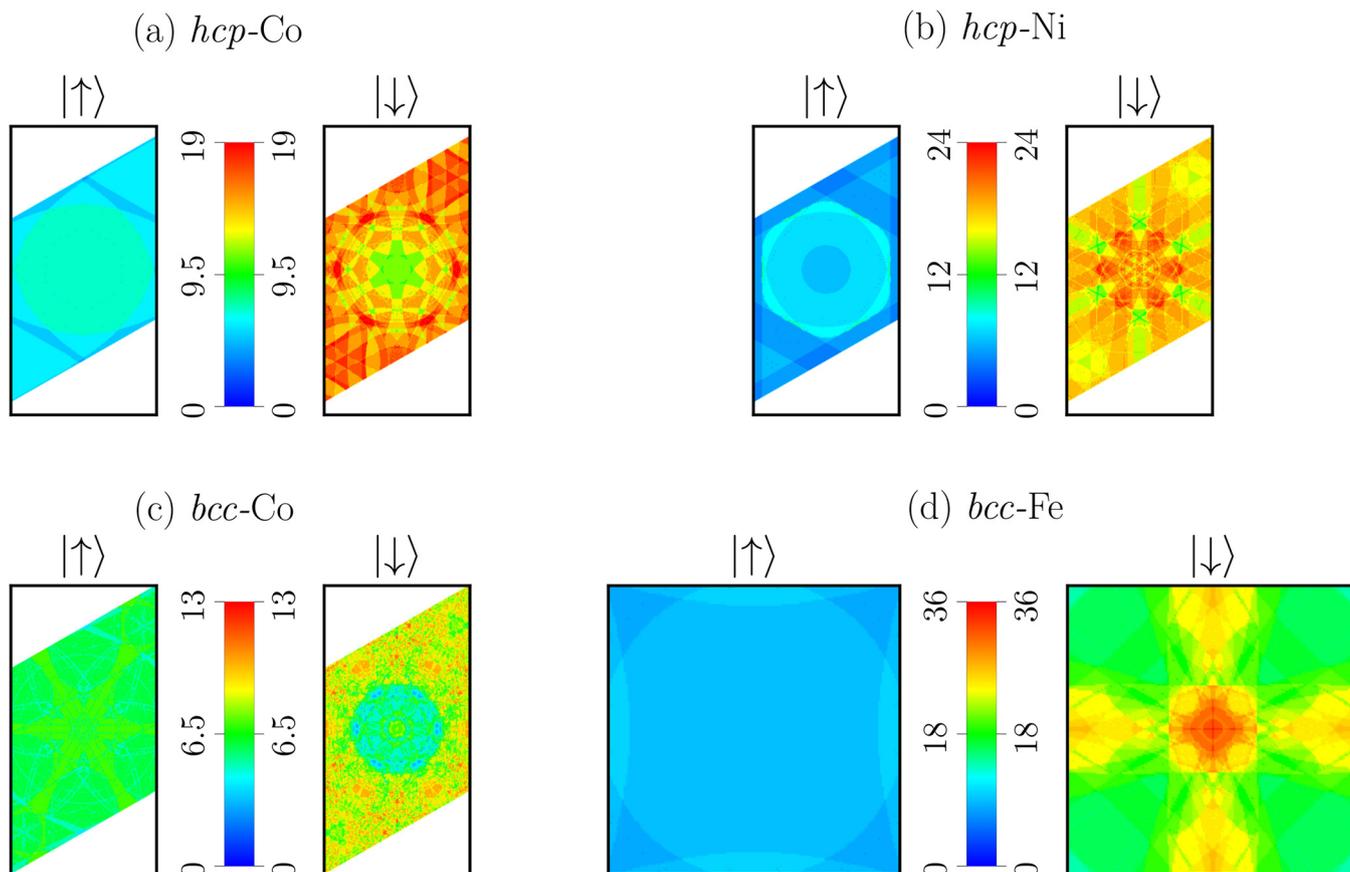


Fig. 4 Momentum-dependence of the number of majority and minority spin transport channels (along the [0001], [0001], [111], and [001] directions, respectively) at  $E_F$  in (a) *hcp*-Co, (b) *hcp*-Ni, (c) *bcc*-Co, and (d) *bcc*-Fe. The color range reaches up to the maximum of available transport channels. The results refer to simulation cells of 36 atoms.

Fig. 5 shows the resultant  $T_P(E_F)$  and  $T_{AP}(E_F)$  in the BZ. For the Co/AlP/Co junction,  $T_P(E_F)$  is high in a broad circular region around the  $\Gamma$ -point in the spin majority channel and in narrow regions in the spin minority channel, while  $T_{AP}(E_F)$  is high only in narrow regions in both spin channels. For the Ni/AlP/Ni junction, both  $T_P(E_F)$  and  $T_{AP}(E_F)$  are high in circular regions around the  $\Gamma$ -point, and  $T_{AP}(E_F)$  is additionally high in circular regions close to the ends of the longer diagonal of the BZ in the spin minority channel. For the Co/GaN/Co junction, both  $T_P(E_F)$  and  $T_{AP}(E_F)$  are high in circular regions around the  $\Gamma$ -point in both spin channels. Finally, for the Fe/GaN/Fe junction, high values of both  $T_P(E_F)$  and  $T_{AP}(E_F)$  are found in large parts of the BZ in both spin channels.

Fig. 6(a and b) shows for the AlP-based junctions that  $T_{P/AP}(E)$  drops around  $E_F$  by about three orders of magnitude. For the Co/AlP/Co junction, the majority spin channel contribution to  $T_P(E)$  with  $\Delta_1$  symmetry dominates over the minority spin channel contributions to  $T_P(E)$  with  $\Delta_1$  and  $\Delta_5$  symmetries in the range  $-1 \lesssim E - E_F \lesssim 0.5$  eV and the minority spin channel contributions to  $T_{AP}(E)$  with  $\Delta_1$  and  $\Delta_5$  symmetries dominate over the majority spin channel contribution to  $T_{AP}(E)$  with  $\Delta_1$  symmetry in the range  $0 \lesssim E - E_F \lesssim 1$  eV. The low  $T_{AP}(E)$  gives rise to a maximal TMR of  $\sim 200\%$  at  $E_F$ . For the

Ni/AlP/Ni junction, the minority spin channel contributions to  $T_P(E)$  with  $\Delta_1$  and  $\Delta_5$  symmetries dominate over the majority spin channel contribution to  $T_P(E)$  with  $\Delta_1$  symmetry in the range  $-1 \lesssim E - E_F \lesssim -0.5$  eV and the minority spin channel contributions to  $T_{AP}(E)$  with  $\Delta_1$  and  $\Delta_5$  symmetries dominate over the majority spin channel contribution to  $T_{AP}(E)$  with  $\Delta_1$  symmetry in the range  $-0.5 \lesssim E - E_F \lesssim 0$  eV, giving rise to a maximal TMR of  $\sim 120\%$  at  $E - E_F = -0.8$  eV.

Fig. 6(c and d) shows for the GaN-based junctions that  $T_{P/AP}(E)$  drops around  $E_F$  by about two orders of magnitude. For the Co/GaN/Co junction, the majority spin channel contribution to  $T_P(E)$  with  $\Delta_1$  symmetry dominates over the minority spin channel contribution to  $T_P(E)$  with  $\Delta_1$  symmetry in the range  $-2 \lesssim E - E_F \lesssim 1$  eV and the minority spin channel contribution to  $T_{AP}(E)$  with  $\Delta_1$  symmetry dominates over the majority spin channel contribution  $T_{AP}(E)$  with  $\Delta_1$  symmetry in the range  $-0.5 \lesssim E - E_F \lesssim 0.5$  eV. The low  $T_{AP}(E)$  gives rise to a maximal TMR of  $\sim 300\%$  at  $E - E_F = -1.4$  eV. For the Fe/GaN/Fe junction, the majority spin channel contributions to  $T_P(E)$  with  $\Delta_2$  and  $\Delta_5$  symmetries dominate over the minority spin channel contributions to  $T_P(E)$  with  $\Delta_1$  and  $\Delta_2$  symmetries in the range  $-3 \lesssim E - E_F \lesssim -1$  eV, the majority spin channel contributions to  $T_P(E)$  with  $\Delta_1$  and  $\Delta_5$  symmetries dominate over the



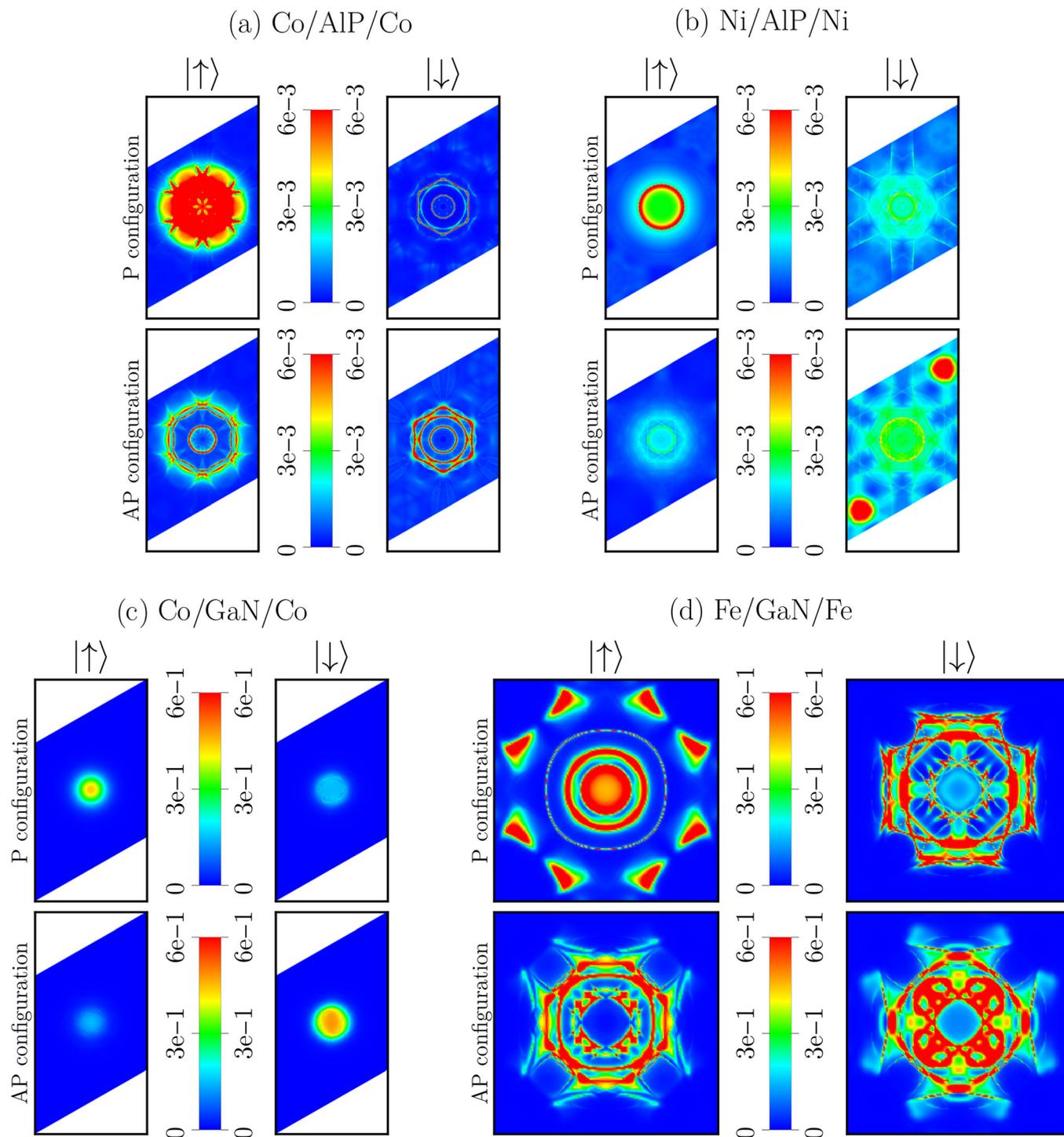
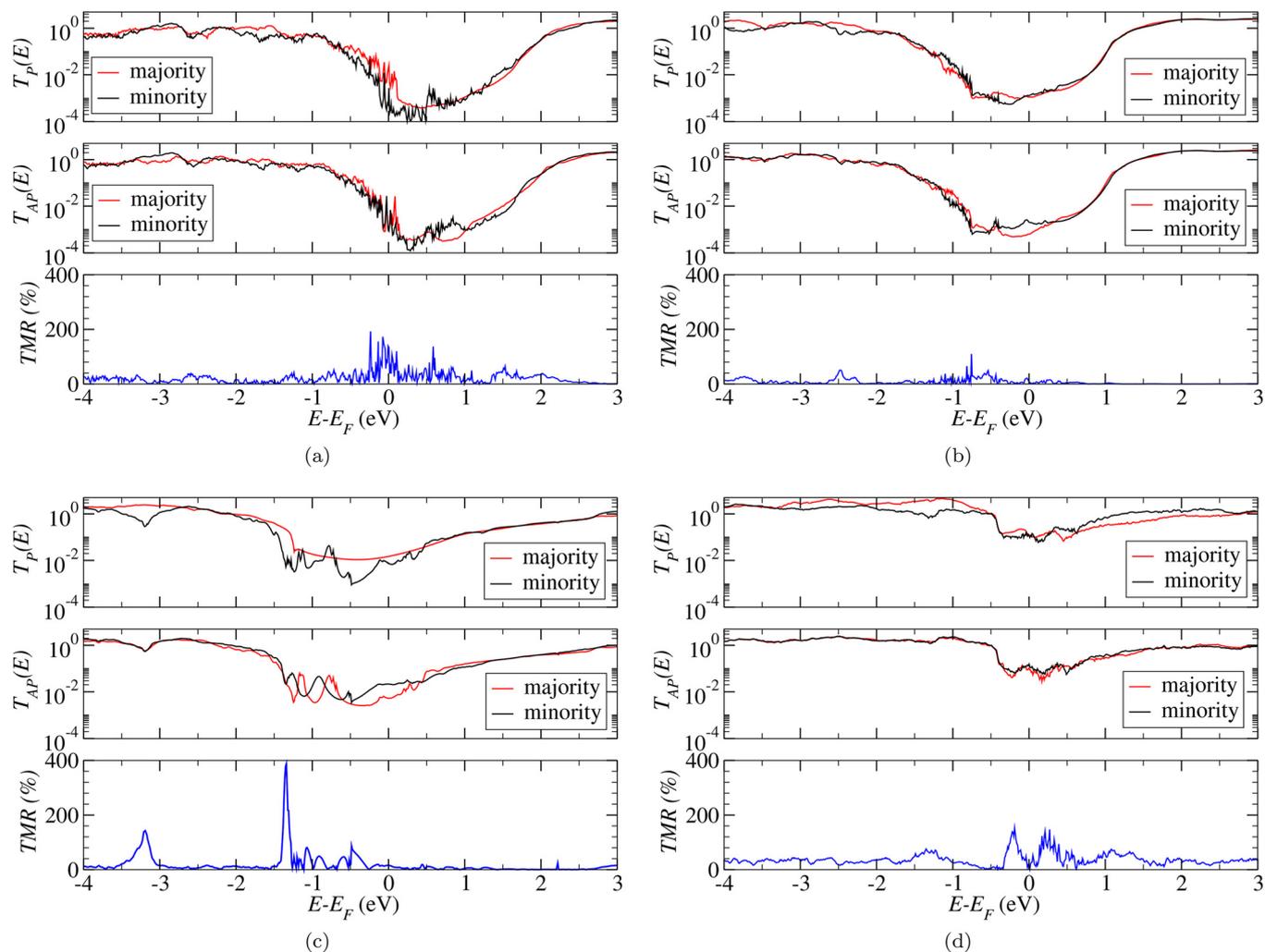


Fig. 5  $T_P(E_F)$  and  $T_{AP}(E_F)$  for the (a) Co/AIP/Co, (b) Ni/AIP/Ni, (c) Co/GaN/Co, and (d) Fe/GaN/Fe junctions.

minority spin channel contributions to  $T_P(E)$  with  $\Delta_2$  and  $\Delta_5$  symmetries in the range  $-1 \lesssim E - E_F \lesssim 0$  eV, and the minority spin channel contributions to  $T_P(E)$  with  $\Delta_1$  and  $\Delta_5$  symmetries dominate over the majority spin channel contribution to  $T_P(E)$  with  $\Delta_1$  symmetry in the range  $0 \lesssim E - E_F \lesssim 2$  eV. Moreover, the majority spin channel contributions to  $T_{AP}(E)$  with  $\Delta_2$  and  $\Delta_5$  symmetries dominate over the minority spin channel con-

tributions to  $T_{AP}(E)$  with  $\Delta_1$  and  $\Delta_2$  symmetries in the range  $-3 \lesssim E - E_F \lesssim -1$  eV, the minority spin channel contributions to  $T_{AP}(E)$  with  $\Delta_2$  and  $\Delta_5$  symmetries dominate over the majority spin channel contributions to  $T_{AP}(E)$  with  $\Delta_1$  and  $\Delta_5$  symmetries in the range  $-1 \lesssim E - E_F \lesssim 0$  eV, the minority spin channel contributions to  $T_{AP}(E)$  with  $\Delta_1$ ,  $\Delta_2$ , and  $\Delta_5$  symmetries dominate over the majority spin channel contribution to  $T_{AP}(E)$  with  $\Delta_1$





**Fig. 6** Transmission coefficients under P (top panels) and AP (middle panels) spin alignments of the electrodes as well as resultant zero bias TMR (bottom panels) as functions of the energy for the (a) Co/AlP/Co, (b) Ni/AlP/Ni, (c) Co/GaN/Co, and (d) Fe/GaN/Fe junctions. The AP spin alignment is obtained by flipping the spin direction in the right hand electrode.

symmetry in the range  $0 \lesssim E - E_F \lesssim 2$  eV, and the majority spin channel contribution to  $T_{AP}(E)$  with  $\Delta_1$  symmetry dominates over the minority spin channel contribution to  $T_{AP}(E)$  with  $\Delta_1$  symmetry in the range  $2 \lesssim E - E_F \lesssim 3$  eV. As a result, we obtain a maximal TMR of  $\sim 150\%$  at both  $E - E_F = -0.2$  and  $0.3$  eV.

## IV. Conclusion

We have explored the possibility of using the optoelectronic materials AlP and GaN as tunnel barriers in the next generation of magnetic tunnel junctions, which would enable the design of hybrid memory/logic components and spin-based displays. As ferromagnetic electrodes, we have considered *hcp*-Co, *hcp*-Ni, *bcc*-Co, and *bcc*-Fe. Analysis of the complex wave vectors of AlP and GaN has enabled us to establish the high transmission regions of the BZ and analysis of the complex band structures has provided us with the symmetries of the

Bloch states dominating the transmission. For both semiconductors, both the valence band edge (dominated by  $p_z$  orbitals) and the conduction band edge (dominated by  $s$  orbitals) are located at the  $\Gamma$ -point. The transmission probability turns out to be high for Bloch states of  $\Delta_1$  symmetry. The Co/AlP/Co, Ni/AlP/Ni, Co/GaN/Co, and Fe/GaN/Fe junctions achieve at zero bias maximal TMRs of  $\sim 200\%$  (at  $E_F$ ),  $\sim 120\%$  (at  $E - E_F = -0.8$  eV),  $\sim 300\%$  (at  $E - E_F = -1.4$  eV), and  $\sim 150\%$  (at  $E - E_F = -0.2$  and  $0.3$  eV), respectively, which demonstrates that they are viable candidates particularly for low power applications.

## Conflicts of interest

There are no conflicts to declare.



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