Co/AIP/Co, Co/GaN/Co as magnetic tunnel junctions

Gokaran Shukla\textsuperscript{1}, Stefano Sauvito\textsuperscript{2}, and Geunsik Lee\textsuperscript{1}

\textsuperscript{1}Department of Chemistry, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea and
\textsuperscript{2}School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland

(Dated: April 1, 2021)

AIP and GaN are wide band-gap semiconductors (SC) uses in opto-electronic industry as light emitting diodes. Here we investigate it as future perspective candidate for insulating barrier in magnetic tunnel junctions. We employ density functional theory for ground state electronic properties and non-equilibrium Green’s function method for quantum transport and examined Co/AIP/Co and Co/GaN/Co MTJs. We find that both AIP and GaN valance band maxima are predominantly made with $p_z$-type orbitals while conduction band minima are $s$-type symmetry. We find that both AIP and GaN filter $\Delta_1$ symmetry of Bloch states at $\Gamma$-point and transmission coefficient at any energy level in-between the band-gap of materials, is mostly driven by $\Delta_1$ symmetry of Bloch states tunnel via $\Gamma$-point in first Brillouin zones. We find large magneto-resistance $\sim 300\%$ in Co/AIP/Co MTJs at zero-bias. In Co/GaN/Co MTJs we find $\sim 300\%$ TMR at 1.25 eV below the Fermi energy ($E_F=1.25$ eV), while $\sim 10\%$ TMR around $E_F$ in zero-bias calculations. We notice that both majority and minority $\Delta_1$ symmetry of Bloch states with rather different $spd$-orbitals compositions tunnel in Co[0001]/AIP[0001] MTJs and exhibit non-zero TMR, whereas in Co[111]/GaN[0001] MTJs, the both majority and minority $\Delta_1$ symmetry of Bloch states with different energy-gradient tunnels at Fermi energy level along [111] transport direction. Our work accentuate the process for systematic, efficient, accurate and versatile framework to design the semiconductors based MTJs for low power electronics.

PACS numbers:

I. INTRODUCTION

The first evidence of anisotropic magneto-resistance is established by Lord Kelvin in iron\cite{19}. Then in early seventies tunneling magnetoresistance is reported in Fe/Ge/Co MTJs by Julieri\cite{20} at low temperature (4K). Later GMR discovery by Fert\cite{21} and Grüneisen\cite{22} expedite this field which is now called as spintronics. In GMR, non-ferromagnet metal such as Pt or Cu is sandwiches between two ferromagnetic electrodes. Such magnetic devices offer two unique resistance states dependent on the spin alignment of two electrodes. In TMR based MTJs, non-ferromagnet stack of GMR device is replaced by insulating materials across which electron tunnel and encounter different resistance which is then decided by the symmetry of Bloch states and magnetic moments alignment of electrodes. Julliere invoke a simple formula for TMR using spin-polarized density of states of ferromagnetic electrodes and defines $TMR = 100 \times \frac{D_{P} - D_{A}}{D_{P} + D_{A}}$, where $P_{1}$ ($P_{2}$) are the spin-polarized density of states of left (right) electrodes. The polarized density of states is generally defined as $p = \frac{D_{\sigma}}{D_{1} + D_{2}}$, with $D_{\sigma}$ being the DOS of the majority ($\sigma = \uparrow$) and minority ($\sigma = \downarrow$) electrons. If one uses optimum definition of $TMR = \frac{P_{\uparrow} - P_{\downarrow}}{P_{\uparrow} + P_{\downarrow}}$, where $P_{\uparrow}$ ($P_{\downarrow}$) being the current for PA (AP) configuration, then Julliere’s theory predict TMRs $\sim 60-70\%$ for magnetic transition metals based MTJs irrespective of the electronic properties of insulators, which is clearly oblique to various experimental result. After that in early nineties it is established that $\sim 20\%$ TMR is attainable with amorphous Al$_2$O$_3$ insulating barrier at room temperature\cite{23}. Later it is established that spin polarized current is not always proportional to density of states and in many cases it is very system dependent\cite{24}. The major break through discern in early 2000 when Butler\cite{25} and Mathon\cite{26} independently demonstrated that in epitaxial junction an arbitrary large TMR is possible. In epitaxial MTJs, the transverse wave vector $k_{\perp}$ remains conserve during tunneling and electron encounter different resistance based on orbital symmetry of wave-function. Soon such prediction is confirmed in FeCoB[001]/MgO[001]/FeCoB[001] based MTJs with reported TMR $\sim 230\%$ at room temperature\cite{27,28,29}. After that Fe/MgO based MTJs enter in main-stream application such as in magnetic read-head, spin torque oscillators (STOs), magnetic random access memory (MRAM). Although experimental TMR analysis is done with various semiconductors yet comprehensive theoretical investigation using ($k_x, k_y$) decay plot and complex-band which is nothing but the solution of secular-band equation extended over to complex wave vector is missing from literature. Complex-wave-vector determines the decay length of Bloch states with different wave-function symmetries inside the insulating barrier region which need to be account in-order to explain otherwise various unexplained or abnormal experimented result in spin dependent semiconductor based magnetic tunnel junction. Furthermore it is of interest of magnetic-devices to perform theoretical study on SC based MTJs comprehensively in-order to obtain deeper insight which then can use to design new MTJs or to manipulate spin moment of magnetic quantum bit using spin-polarized current. In spite of the fact that concept of orbital- spin-symmetry filtering is applicable in various insulating stack such as Fe(100)/HfO$_2$, Co(0001)/SiO$_2$\cite{30},...
STO/BaTiO$_3$, Cu/EuO, Co(0001)/h-BN, Co$_2$MnSi/MgF$_2$, however, only FeCoB/MgO based MTJs is currently in use in various mainstream applications. This can be ascribed to various reasons including boron assisted epitaxial growth of Fe/MgO interface which then oblige for high transmission to spin-polarized current. It is known that propensity to generate spin-polarized current and detect it indubitably is the principal requirement for any spintronics devices. Currently Fe/MgO based MTJs play a central role at this front. However, Fe/MgO based MTJs carry certain disadvantages at fabrication level where four fold symmetry MgO need to be grown on six fold fcc[111] plane of lattice constant by 3.75 Å for epitaxy using 2×3 [0001] plane match with hcp-[111] plane. GaN exhibit wurzite crystalline structure in bulk with in plane lattice constant (a) 3.19 Å while out of plane (c) is 5.19 Å. We extend in plane lattice constant to 3.34 Å and construct 2×2 [0001] plane match with 3×3 hcp-Co [0001] plane for epitaxy. In Co/AIP MTJs the both left and right interfaces are nearly-symmetric (strictly it is asymmetric) where FM Co encounter P both at other interface. Such stacks are decided after employing thermodynamics Gibb’s formation energy of compositions. In contrast GaN MTJs is perfectly asymmetric exposing left interface as Co/Ga while right-one is as Co/N. In this case, inversion symmetries is broken which will then predominantly uplift the spin degeneracy in anti-parallel configuration transmission $T(E)$ coefficient. We then take 22.5 Å and 16.1 Å thick AIP and GaN as an insulating barriers for Co/AIP and Co/GaN based MTJs for spin dependent quantum transmits.

We employ smeagol$^{22,23}$ code which ingrain non-equilibrium Green’s function method for transport calculation while siesta based DFT for ground state electronic structures. In NEGF formalism the left and right lead coupling matrix with scattering-device-region is described by complex- self energy density matrix $\sum_{L,R}(E)$. The complex self-energy add to bare surface Green’s function of device region ground state Hamiltonian $H_C$ and transformed it as an effective Hamiltonian of device under semi-infinite leads contacts. One can then conclude that over-all effect of semi-infinite leads on device regions is to modify the device region Hamiltonian as an effective Hamiltonian which then goes into SMEAGOL for effective device regions Green’s function calculations. One can then write effective Green’s function of device regions, $G_C(E)$ as,

$$ G_C(E) = \lim_{\eta \to 0} \frac{1}{E+i\eta-H_C(E)-\sum_{L}(E)-\sum_{R}(E)^{-1}}, \quad (1) $$

where $\sum_{\lambda} (\lambda = L, R)$, $H_C$ is Hamiltonian of scattering region and $H_{SC}$ is coupling Hamiltonian matrix between leads and scattering region. It is to note that an effective Hamiltonian should only be used for scattering region
Green’s function calculations and not for eigenvalue and eigenvectors due to complication of it any physical realistic interpretation. The resulting \( G_c(E) \) is then finite and hermitian at equilibrium with associated density matrix, 

\[
\rho = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dEG_c^\dagger(E),
\]

where \( G_c^\dagger(E) \) is a lesser Green’s function which generally defines as \( G_c^\dagger(E) = iG_c(\sum_{L,R}f_{L,R}\Gamma_{L,R})G_c(E) \). \( f_{L,R} \) is Fermi-Dirac distribution for left and right leads, \( \Gamma_{L,R}(E) \) is the coupling matrix between leads and scattering region mathematically defines as \( \Gamma_{L,R}(E) = \sum_{L,R}(E) - \sum_{m} \). We define spin-dependent zero bias transmission coefficient \( T(E) \) as

\[
T^\sigma(E) = T_r[\Gamma_r^\dagger(E)G_r^–(E)\Gamma_r^0(E)G_r^+\sigma(E)],
\]

for SMEAGOL which then calculate voltage dependent spin polarized current using Landauer-Büttiker formalism as

\[
I^\sigma(V) = \frac{e}{h} \int_{-\infty}^{\infty} dE T^\sigma(E;V)[f_L - f_R],
\]

where \( h \) the Plank constant, \( e \) is electron charge, \( \sigma(\uparrow, \downarrow) \) for spin moment, \( T^\sigma(E;V) \) is energy and voltage dependent transmission coefficient. \( f_L \) (\( f_R \)) the Fermi-Dirac distribution function of left (right) electrode which is then evaluated at \( E - \mu_L \) (\( E - \mu_R \)), where \( \mu_L/R = E_F \pm \frac{eV}{\hbar} \) is the chemical potential of left/right electrode under bias voltage \( V \). Since the junction is translationally invariant along the transverse direction, we can integrate transmission coefficient \( T^\sigma(E;V) \) across a plane perpendicular to the transport direction in first Brillouin zone. Mathematically \( T^\sigma(E;V) \) it is defined as

\[
T^\sigma(E;V) = \frac{1}{\Omega_{BZ}} \int_{BZ} d\mathbf{k}_\parallel T^\sigma_{\mathbf{k}_\parallel}(E;V),
\]

where \( \Omega_{BZ} \) is volume of first Brillouin zone. The transport calculation is performed after converging charge density on \( 8 \times 8 \times 1 \) k-grid point with density-matrix \( (dm) \) tolerance \( 10^{-4} \). Transmission coefficient in then calculated using \( 50 \times 50 \times 1 \) mesh points. We also checked transmission coefficient on \( 100 \times 100 \times 1 \) mesh without notice any significant change in \( T^\sigma(E;V) \) or the TMR.

III. RESULTS AND DISCUSSION

A. AIP and GaN as tunnelling barriers

AIP and GaN are wide band-gap semiconductors use in opto-electronics industries as light emitting diodes. GGA with PBE xc-functional return direct band-gap \( 2.2 \) eV for AIP at \( \Gamma \) point. This is very close to the experimented band-gap of \( 2.5 \) eV. In case of GaN with LDA functional we get direct band-gap \( 2.2 \) eV which is underestimated by \( 1.0 \) eV with experiment. We then corrected GaN band-gap using self-interaction corrections method, which return relatively better value \( 2.6 \) eV. It is to note that correction in band-gap will only affect the magnitude of transmission coefficient \( T(E) \) while physics associated to problem remains unchanged. We then investigated \( k_z = ik \) complex wave vector decay in insulating barrier region as a function of incident energy \( E \) and transverse wave -vector \( \mathbf{k}_\parallel \). The complex wave-vector \( k \) in insulating barrier regions is generally defines as \( k = \sqrt{(2m/\hbar^2)(V - E) + k_\parallel^2 - \frac{\langle \phi | \frac{\partial^2}{\partial x^2} + V_0 \phi | \phi \rangle}{\langle \phi | \phi \rangle}} \). It is to note that last term in \( k \) (Laplacean term) result due to oscillation of wave-function in a plane perpendicular to the transport directions. Higher angular momentum wave-function will then encounter large decay coefficient \( k \) in insulating barrier regions. The transmission coefficient is then expected to decay with insulating barrier thickness \( d \) as \( T(E,\mathbf{k}_z) \sim T_0(E,\mathbf{k}_z)e^{-2\kappa(E,\mathbf{k}_z)d} \), where \( T_0(E,\mathbf{k}_z) \) depends on the atomic composition and nature of interface (epitaxial or amorphous). We then plot \( \kappa(E_F,\mathbf{k}_z) \) in 2D Brillouin zone traverse by the transverse wave-vector \( \mathbf{k}_z \) and established high transmission regions in tunneling current. The outcome of such analysis are presented in Fig. 1 for AIP and in Fig. 2 for GaN.

![Fig. 1](image-url)  
**FIG. 1:** The heat colour plots represents the wave-function decay coefficient, \( \kappa(E_F,\mathbf{k}_z) \), as a function of the transverse wave-vector, \( \mathbf{k}_z \), for AIP. The transmission calculations is done with \( E_F \) in the middle of the band gap. The black boxes encloses \( \Gamma \) centered 2D Brillouin zones while colour code blue to green to red represent decay coefficient \( \kappa \) as it gets larger. \( k \) is plotted in linear scale with the following limit: AIP \( \kappa_{\min} = 2.2 \) A\(^{-1}\), \( \kappa_{\max} = 3.1 \) A\(^{-1}\).

Fig.1 and Fig.2 show that tunneling electrons have minimum decay coefficient at \( \Gamma \) point in first Brillouin zone. The \( \Gamma \) point corresponds to the situation when tunneling electrons approaches along normal to the plane of insulating barrier. In such situation drift along transverse direction is absent which then assisted in tunneling by reducing the effective barrier thickness encoun-
FIG. 2: The heat colour plots of the wave-function decay coefficient, \( \kappa(E_F, k) \), as a function of the transverse wave-vector, \( k \parallel \), for GaN. Calculations is carried out for \( E_F \) placed in the middle of the band gap. The black boxes mark the 2D Brillouin zones and the colour code is blue to green to red as \( \kappa \) gets larger. The decay coefficient is plotted in linear scale with the following limit: \( \kappa_{\text{min}} = 1.04 \text{ Å}^{-1} \), \( \kappa_{\text{max}} = 3.63 \text{ Å}^{-1} \).

FIG. 3: Real (right-hand side panel) and complex (left-hand side panel) band structure of AIP calculated at the \( \Gamma \) point in the 2D transverse Brillouin zone. The symmetry labels, \( \Delta_n \), have been described in the text and the Fermi energy is taken at \( E - E_F = 0 \). The valance band maxima is predominantly \( p_z \) type while conduction band-minima is made with \( s \)-type orbitals.

B. Symmetry of Bloch states

Generally the symmetry of Bloch states is assigned after looking at their atomic composition once projecting it along transport direction. In particular, \( \Delta_1 \) symmetry correspond to \( s \), \( d_{3z^2-r^2} \) and \( p_z \)-type orbitals having zero angular momentum along transport direction. In contrast \( d_{xz} \), \( d_{yz} \), \( p_x \) and \( p_y \) are assigned as \( \Delta_5 \) symmetry. Finally we assign \( \Delta_2 \) to \( d_{xy} \) and \( \Delta_2 \) to \( d_{2z^2-r^2} \) orbitals. The real and complex-band structures calculated at \( \Gamma \) point in 2D transverse Brillouin zones for AIP and GaN are presented in Fig. 3 and Fig. 4 respectively. The symmetry of different bands are mentioned in figure. Also, in both Fig. the evanescent states with decay coefficient \( k \) is smoothly connect the balance band maxima to conduction band minima. We did not find any spurious ghost states in complex bands which some time appear with flat energy dispersion relations due to non-orthogonal orbital basis set27.

Both semiconductors exhibit very similar electronic characters. In particular, both filter \( \Delta_1 \) symmetry of...
FIG. 4: Real (right-hand side panel) and complex (left-hand side panel) band structure of GaN calculated at the Γ point in the 2D transverse Brillouin zone. The symmetry labels, $\Delta_n$, have been described in the text and the Fermi energy is taken at $E - E_F = 0$. The valence-band maxima of GaN are predominantly $p_z$ type while conduction-bands minima are with $s$-type orbitals.

Bloch states at Γ point and have very similar bandgap. $\Delta_1$ symmetry of Bloch states exhibit slowest decay rate and connect valance band-maxima to the conduction band-minima with smallest curvature. Moreover both materials valance band maxima are made with predominantly $p_z$ type orbitals while conduction bands minima are with $s$-type symmetry. One more band with $\Delta_5$ symmetry is also present at valance band maxima, however it have large decay coefficient $k$ exhibit large curvature radius. It shall not participate in transmission unless Fermi level of magnetic tunnel junction is pinned very close to valance-bands maxima.

C. Ferromagnetic electrodes

We investigated two magnetic tunnel junctions using hcp-Co as ferromagnetic electrodes and different transport directions. For high TMR, ideal ferromagnet should exhibit only one spin symmetry of Bloch state at Fermi energy which should then match with insulating barrier symmetry at Γ-point along transport direction. In such cases ferromagnet/insulator stack behaves like a half metal in which available states tunnel across the insulating barrier and exhibit exponential thickness dependent magnetoresistance. The exact situation arises in Fe/MgO MTJs in which iron supply majority $\Delta_1$ and both spin $\Delta_5$ states along [001] transport direction. MgO filter $\Delta_1$ symmetry at Γ-point and exhibit enormous $\sim 10,000\%$ TMR in Fe/MgO MTJs.

The real band structure of hcp-Co is plotted in Fig. 5 along [0001] direction. The bcc-Co bands is plotted in Fig. 6 along [111] direction. We find that both ferromagnet supply the required symmetry of Bloch states along transport directions. In case of hcp-Co majority $\Delta_2'$, minority $\Delta_2$ and $\Delta_5$ symmetries are crossing at Fermi energy. These spin bands are shifted due to exchange field, still exhibit high transmission in both spin channel. However, we know that Co is a strong ferromagnet with fully filled majority $d$ band, the majority $\Delta_2$ band at $E_F$ need to be attributed to hybrid $spd$ states in which $d$ orbital content is expected to be different than from minority counterpart.

The case of bcc-Co along [111] is quite different. At $E_F$, both majority and minority sub-bands with $\Delta_1$ symmetry are available along transport direction. The majority and minority sub-bands dispersion relation are shifted due to exchange field exhibit different curvature (effective mass) and gradient (group velocity) at Fermi energy. The effect of these two will be resulted with high transmission $T(E)$ for one spin channel over the other in transport calculations. There are another minority sub-bands with $\Delta_5$ symmetry are available near Fermi energy.

FIG. 5: Real band structure of hcp Co is plotted along the [0001] transport direction. The majority spin sub-band is in red and the minority one in black. The Bloch state symmetry is assigned to both majority and minority sub-bands.
Next we move our attention to transmission coefficient $T(E)$ in parallel configuration (panel (a) in Fig. 7). One can see that majority spin channel is dominating over minority spin transmission in entire energy window from -0.5 to 2.5 eV. The very similar trend is present in anti-parallel configuration (panel (b)) except around the Fermi energy where fluctuation in minority spin channel is noticed. In between -0.5 eV to $E_F$, the majority $\Delta_2^\prime$ symmetry of states dominates over minority $\Delta_2^\prime$ states. Both majority and minority sub-bands are shifted due to exchange-energy and exhibit rather different curvature and energy-gradient in this window. There are only two majority sub-bands with $\Delta_2^\prime$ symmetry are available in between -0.5 to 0 eV energy-range. In contrast there are many minority $\Delta_2^\prime$ sub-bands are available in between -0.5 to 0 eV. The majority sub-bands with relatively higher energy-gradient and smaller radius of curvature (effective mass) in energy-dispersion relations dominate over minority in tunneling till $E_F$. In between 0 to 0.25 eV minority sub-bands with $\Delta_2^\prime$ symmetry reverse it trend and dominate over majority. After that majority sub-bands with large energy-gradient takes over minority $\Delta_2^\prime$ sub-bands until Fermi energy enter into conduction band around $\sim$2.4 eV. We fond robust TMR $\sim$300% at zero energy bias in Co/AIP MTJs. This is promising result for low power spintronics based MTJs.

**D. Tunnel magnetoresistance**

We now turn our attention to the TMR analysis in Co/AIP/Co MTJs. The transmission coefficient as a function of energy is plotted in Fig. 7 for both spin channel in parallel (a) and anti-parallel (b) configurations. Anti-parallel configuration is obtained after spin-moments flipping of right FM electrodes. As it is shown in Fig. 7 the transmission coefficient $T(E)$ is dropped drastically by $\sim$4 order of magnitude in energy regions approximately 2.2 eV wide which is correspond to the sic-corrected band-gap of AIP. In AP configuration (b) $T(E)$ for majority and minority spin are not exact (overlap), although majority (minority) sub-bands electrons from left electrodes tunnel to minority(majority) sub-bands in right electrodes. It is due to the absence of inversion symmetry at interfaces in MTJs. The left interface composed of Co/Al elements while right one is made with Co/P. In MTJs the Fermi level is positioned around 1 eV above the balance band maxima. Also, $T(E)$ plot on logarithmic scale (panel (a) and (b) in Fig. 7) suggest that transmission in both cases (parallel and anti-parallel configuration) is mostly dominated by low lying complex band structure of AIP around $\Gamma$-point. This established the fact that transport in AIP is mostly driven by $\Gamma$ point and it allow $\Delta_1$ symmetry of Bloch states to tunnel faster in insulating barrier regions over the other symmetry of states.

**FIG. 6:** Real band structure of bcc Co is plotted along the [111] transport direction. The majority spin sub-band is in red and the minority one in black. The symmetry of Bloch states is assigned to majority sub-band only. The minority sub-bands too have the same symmetry as the majority ones.

**FIG. 7:** (Colour on line) The logarithmic transmission coefficient as a function of energy is plotted for Co/AIP/Co MTJs. Panel (a) and (b) corresponds to parallel and anti-parallel configuration setup. Anti-parallel spin-direction is obtained by right hand side electrode. $T(E)$ of majority (minority) spins is plotted in red (black). In same energy window the zero-bias TMR is plotted in panel (c).

Next we analyse Co/GaN/Co MTJs which exhibit $\sim$2.5 eV LDA-ASIC energy band-gap with Fermi level lies $\sim$0.5 eV below the conduction band. The various transmission coefficient is shown in Fig. 8 at logarithmic scale. $T(E)$ shows quite complex oscillatory structure in band-gap for both P and AP configurations. In parallel case (see panel (a) Fig. 8) majority $\Delta_1$ band dominates over minority $\Delta_1$, $\Delta_2$ and $\Delta_5$ bands in energy window between $E_F - 2$ to $E_F + 0.5$ eV except at $E_F - 0.7$ eV.
FIG. 8: (Colour on line) Transmission coefficient as a function of energy for the Co/GaN/Co MTJ. The parallel and antiparallel configurations are plotted in panel (a) and (b) respectively. $T(E)$ for the majority (minority) spin is plotted in red (black). For the antiparallel case the spin direction is set by the right-hand side electrode. The transmission coefficient is plotted in logarithmic scale. In the lower panel (c) we present the calculated zero-bias TMR as a function of energy in the same energy window of the transmission coefficients.

where minority band shows higher transmission coefficient with one dominant peak. In AP (panel (b)) the minority $\Delta_1$ bands dominate over majority $\Delta_1$ band in between $E_F - 1.5$ to $E_F - 1.25$ eV, then majority $\Delta_1$ bands till $E_F - 1$ eV. After that minority $\Delta_1$ bands dominate over majority $\Delta_1$ till $E_F - 0.75$ eV. Next majority $\Delta_1$ sub-bands dominate over minority $\Delta_1$ till $E_F - 0.5$ eV. After that minority $\Delta_1$ and $\Delta_2$ sub-bands takes-over majority $\Delta_1$ band till $E_F + 0.5$ eV. It is to note that it is a qualitative explanation because transmission coefficient is not only calculated at $\Gamma$-points but in entire Brillouin zone where different symmetry of Bloch state tunnel with different complex wave-vector $k$ in transport direction. The resulting TMR as a function of energy is then plotted in lower panel of Fig.8 which nicely validated our $T(E)$ analysis. We find a robust TMR reaching upto 300% at $E = E_F - 1.25$ eV. The oscillatory structure of TMR present in between $E_F - 1.5$ to $E_F - 25$ eV is due to the complex-behavior of $T(E)$. Also, Co/GaN MTJs posses no inversion symmetry due to different interfaces at left and right electrodes. At left interface Co face gallium whereas at right interfaces Co encounter nitrogen resulting asymmetric junction which further lift spin-degeneracy and induce structure complexity in $T(E)$ (see Fig.8 panel (b)). The TMR at $E = E_F - 1.25$ eV is significantly larger than that predicted by Juillere formula which confirms that some level of spin filtering is at work around $\Gamma$ point. Therefore we are concluding that Co/GaN/Co can represent a viable alternatives to other spin filtering MTJ stack for opto-electronics industries. However, since spin filtering occurs only in a relatively small energy window ($\sim$ 1 eV) we expect that bias dependence TMR will be rather critical and that small TMR will be noticed for bias larger than 1.4 eV below the Fermi level.

IV. CONCLUSION

In summary, we have explored the possibility of using display materials such as AlP and GaN as a magnetic tunnel barriers for next generation MTJs. Both materials are currently used in the microelectronic and opto-electronics industry so that MTJ based on such semiconductors have the potential for integration in hybrid memory/logic components or spin-polarized based display devices or in magnetic quantum-bit. Both AlP and GaP remain in bulk wurzite crystal structure and generates asymmetric left and right interfaces with cobalt ferromagnet in magnetic tunnel junction. We have performed complex-band structure analysis and identified dominant symmetry of Bloch state tunneling in AlP and GaN insulators. We then performed 2d $(k_x,k_y)$ transmission plot and identified the dominant portion of Brillouin zones where $T(E)$ is relatively large in contrast with other parts. We find that at $\Gamma$-point, both semiconductors valence-band maxima are made from predominantly $p_z$-orbitals whereas conduction-bands minima is with $s$-symmetry. Our complex band-analysis established that electron transmission is high for Bloch states with $\Delta_1$ symmetry which connect valence-band maxima to conduction band-minima at $\Gamma$ point. We have then constructed and investigated Co[0001]/AlP[0001]/Co[0001] and Co[111]/GaN/Co[111] as next generation MTJs for micro/opto-electronic industries. We have found that Co/AlP MTJs filter $\Delta_1$ symmetry of Bloch states and exhibit robust $\sim$300 TMR at zero energy-bias. We notice that hcp-Co supply both spin (majority, minority) with $\Delta_1$ symmetry of states along transport directions. Our non-zero TMR at zero-bias established the fact that spd-orbitals contents in both majority and minority $\Delta_1$ symmetries of states are different due to different amount of hybridization in between complete fill majority 3d-bands with $4s$ states over to partially filled minority 3d-bands resulting robust $\sim$ 300 $\%$ TMR. In Co/GaN case we find that energy dependent transmission coefficient is quite oscillatory in both parallel and anti-parallel configuration. In AP case, the majority and minority transmission coefficient does not overlap due to asymmetry of interfaces present in MTJs. We find that Co/GaN/Co MTJs exhibit relatively smaller $\sim$10$\%$ TMR around $E_F$, but robust 300$\%$ TMR at $\sim$1.25 eV below the Fermi energy around $E_F - 1.25$ eV. Our work has demonstrated that Co/AlP/Co and Co/GaN/Co MTJs, are a viable candidates for next generation MTJs for low power micro/opto-electronics industries. Although for high performance junctions one probably has to search different magnetic electrodes (2d
ferromagnets, Heusler alloys) than simple transition metals.

**Acknowledgments.** This work is supported by the National Research Foundation of Korea (Basic Science Research Program: 2021R1A2C1006039) and UNIST Supercomputing Center.

1. Magnetoresistance in metals, A.B. Pippard (1989)
2. M.N. Baibich, J.M. Broto, A. Fert, F.N. van Dau, F. Petroff, P. Eitene, G. Greuzet, A. Friederich and J. Chazelas, Phys. Rev. Lett. 64, 2472 (1988).
3. G. Binasch, P. Gru¨nberg, F. Saurenbach and W. Zinn, Phys. Rev. B 39, 4828 (1989).
4. M. Julliere, Phys. Lett. A 54, 225 (1975).
5. T. Miyazaki and N. Tezuka, J. Magn. Magn. Matter. 139, L231 (1995).
6. J.S. Moodera, L.R. Kinder, T.M. Wong and R. Meservey, Phys. Rev. Lett. 74, 3273 (1995).
7. I.I. Mazin, Phys. Rev. Lett. 83, 1427 (1999).
8. W.H. Butler, X.-G. Zhang, T.C. Schulthess and J.M. Maclaren, Phys. Rev. B 63, 054416 (2001).
9. J. Mathon and A. Umerski, Phys. Rev. B 63, 220403 (2001).
10. S.S.P. Parkin, C. Kaiser, A. Panchula, P.M. Rice, B. Hughes, M. Samant and S.H. Yang, Nature Mater. 3, 862 (2004).
11. S. Yuasa, T. Nagahama, A. Fukushima, Y. Suzuki and K. Ando, Nature Mater. 3, 868 (2004).
12. Handbook of Spin Transport and Magnetism, Eds. E.Y. Tsymbal and I. Zutic, Chapman and Hall/CRC (2011).
13. M. Tanaka and S. Ohya Comp. Sci. Tech. 6, 540 (2011).
14. G. Shukla, T. Archer and S. Sanvito, Phys. Rev. B 95, 184410 (2017).
15. N.M. Caffrey, T. Archer, I. Rungger and S. Sanvito, Phys. Rev. Lett. 109, 226803 (2012).
16. N. Jutong, I. Rungger, C. Schuster, U. Eckern, S. Sanvito and U. Schwingenschlögl, Phys. Rev. B 86, 205310 (2012).
17. S.V. Faleev, S.S.P. Parkin and O.N. Mryasov, Phys. Rev. B 92, 235118 (2015).
18. H.X. Liu, Y. Honda, T. Taira, K.I. Matsuda, M. Arita, T. Uemura and M. Yamamoto, Appl. Phys. Lett. 101, 132418 (2012).
19. S.M. Bhagat and P. Lubitz, Phys. Rev B 10, 179 (1974).
20. J.M. Soler, E. Artacho, J.D. Gale, A. Garcia, J. Junquera, P. Ordejón and D. Sánchez-Portal, J. Phys.: Condens. Matter 14, 2745 (2002).
21. D.M. Ceperly and B.J. Alder, Phys. Rev. Lett. 45, 566 (1980).
22. A.R. Rocha, V.M. Garcia Suarez, S. Bailey, C.J. Lambert, J. Ferrer and S. Sanvito, Nature Mater. 4, 335 (2005).
23. A.R. Rocha, V.M. Garcia Suarez, S. Bailey, C.J. Lambert, J. Ferrer and S. Sanvito, Phys. Rev. B 73, 085414 (2006).
24. I. Rungger and S. Sanvito, Phys. Rev. B 78, 035407 (2008).
25. C.D. Pemmaraju, T. Archer, D. Sánchez-Portal and S. Sanvito, Phys. Rev. B 75, 045101, (2007).
26. A. Filippetti, C.D. Pemmaraju, S. Sanvito, P. Delugas, D. Puggioni and V. Fiorentini, Phys. Rev. B 84, 195127 (2011).
27. F. Sacconi, J.M. Jancu, M. Povolotskyi and A. Di Carlo, IEEE Trans. El. Dev. 54, 3168 (2007).