First-principles spin-transfer torque in CuMnAs|GaP|CuMnAs junctions

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We demonstrate that an all-antiferromagnetic tunnel junction with current perpendicular to the plane geometry can be used as an efficient spintronic device with potential high-frequency operation. By using state-of-the-art density functional theory combined with quantum transport, we show that the Néel vector of the electrodes can be manipulated by spin-transfer torque. This is staggered over the two different magnetic sublattices and can generate dynamics and switching. At the same time the different magnetization states of the junction can be read by standard tunneling magnetoresistance. Calculations are performed for CuMnAs|GaP|CuMnAs junctions with different surface terminations between the antiferromagnetic CuMnAs electrodes and the insulating GaP spacer.

We find that the torque remains staggered regardless of the termination, while the magnetoresistance depends on the microscopic details of the interface.

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Antiferromagnetic (AF) materials are magnetically ordered compounds where two or more spin sublattices compensate each other, resulting in a vanishing macroscopic magnetization. As a consequence, an antiferromagnet does not produce stray field, and closely separated AF nanostructures are not interaction. As a consequence, an antiferromagnet does not produce stray field, and closely separated AF nanostructures are not interaction. In addition, the typical time scale for the dynamics of the antiferromagnetic order parameter, the Néel vector, is set by the AF resonance frequency, which is typically much larger than that of a ferromagnet, and may approach the THz range [1].

We consider the two CuMnAs|GaP|CuMnAs stacks depicted in Fig. 1. These are built along the CuMnAs [001] direction with the GaP spacer taking a zincblende structure. In both cases CuMnAs is terminated at the Cu plane and the two electrodes are atomically mirror symmetric with respect to the central (x-y) plane in the junction. The spacer can then be terminated either at the Ga plane (GPG junction) or at the P one (PGP). In both cases the total number of atoms in the junction supercell is the same, 49 atoms. The different terminations of the spacer result in interfaces where P binds on top to the Cu surface in PGP, while Ga is in hollow site in GPG [3,4] (see also the Supplemental Material (SM) [7]).

The local spin-density approximation (LSDA) is able to reproduce the experimentally observed AF structure of CuMnAs [3] in its tetragonal phase for the experimental lattice parameters. Both the GPG and the PGP junctions consist of three CuMnAs unit cells on each side of a 3-unit-cell-long GaP spacer region. In addition, there is an extra Ga/P layer at one of the interfaces which makes the junctions more symmetric. The whole stacks are relaxed in the z direction within LSDA using periodic boundary conditions in all directions with the SIESTA [8] code. After the geometry optimization, the z coordinates of all atoms in both junctions are further symmetrized with respect to the junction center, with the intention to suppress additional geometry-driven asymmetry effects to the transport properties. In the final geometries, the lead atoms map ideally onto the same species upon reflection in the (x-y) plane through the central atom, and the same is true also for the z coordinates of the spacer atoms, but their corresponding x and y coordinates do not match as the zincblende lattice lacks such a symmetry. In the GPG junction the Cu-Ga distance along the z axis is 1.75 Å for both interfaces, while in the PGP junction the Cu-P distance is 2.16 Å for both interfaces. The total length of the junction is 54.5 Å for the GPG and 54.9 Å for the PGP.

Electron transport through the junctions is described by the Keldysh nonequilibrium Green’s function (NEGF) method as implemented in the SMEAGOL code [9–11]. We consider a steady-state formulation of the STT analogous to that described in Ref. [12]. The key points of our STT implementation...
The coordinate system is chosen such that the $\sigma$ potential (carrying a spin) are described in the SM [7]. The STT at each atomic site $\sigma$ potential ($\Delta_{ij}$) is uniformly distributed in the lead [14], but this picture breaks down in the case of multichannel conductance. Most importantly, the staggered property of the STT is observed in both junctions, which is crucial for the manipulation of the AF order parameter by currents, appears to be a robust property of the AF junctions, and it is weakly affected by the chemistry of the interfaces.

The magnitude of the STT we find at the interfacial Mn layers despite the limiting size of the MTJ stacks considered here, this provides clear indications of decay but also saturation of the staggered in-plane STT in the AF lead away from the interface. This behavior of the STT is similar to what has been found by first-principles calculations in AF spin valves [13] and attributed to the interference of multiple open channels with different $k_z$ at the Fermi level. It had been previously demonstrated that in the limit of a single open channel, in model AF junctions, the nonequilibrium spin density ($\sigma_{\alpha i}^0$) is uniformly distributed in the lead [14], but this picture breaks down in the case of multichannel conductance. Most importantly, the staggered property of the STT observed in both junctions, which is crucial for the manipulation of the AF order parameter by currents, appears to be a robust property of the AF junctions, and it is weakly affected by the chemistry of the interfaces.

We evaluate the atomically resolved SSTk in the right-hand-side lead (RL) for the largest misalignment of $90^\circ$ between the two lead order parameters, i.e., for the Mn spins in the left-hand-side lead (LL) oriented along the $y$ axis, while the RL spins are rotated by $90^\circ$ about the $z$ axis starting from the P state, hence the order parameter in RL is now along $x$ (Fig. 2(a)). The local exchange field $\Delta_{ij}$ within LSDA shows a very similar staggered distribution (not shown here) and the resulting STT in the RL is also staggered. STT is maximal at the very first Mn layer and then decreases in magnitude in the following Mn layers. Despite the limiting size of the MTJ stacks considered here, this provides clear indications of decay but also saturation of the staggered in-plane STT in the AF lead away from the interface.
in the P state: (a), (b) The PDOS of atoms in the (C \rightarrow R) half of the junction. The atom indexes are the same as in Fig. 2. Note that the black curves correspond to the atom (P or Ga) in the very center of the junctions. (c) and (d) show the spectrum of the total transmission in both the P and AP state, while in (e) and (f) the TMR is defined as TMR = (t_π - t_{\text{AP}})/(t_π + t_{\text{AP}}).

Let us now investigate in more detail the electronic and transport properties of each junction in its collinear (P or AP) state. The atomically projected density of states (PDOS) [7] in transport properties of each junction in its collinear (P or AP) state, while in (e) and (f) the TMR is defined as TMR = (t_π - t_{\text{AP}})/(t_π + t_{\text{AP}}).

For further insight we compare the GPG and PGP transmissions \( t_k \) at the Fermi level as a function of the transverse \( k_{\perp} = (k_x, k_y) \) vector resolved over the entire first Brillouin zone (BZ) (Fig. 4). We note that in both cases there are vast regions of the BZ, where \( t_k = 0 \) (blue areas in the transmission panels). This is a direct consequence of the low DOS in the CuMnAs electrodes around \( E_F \). In fact, in Fig. 4(a) one can directly observe that the regions of \( k \) space with \( t_k = 0 \) essentially correspond to regions where there are no open scattering channels at \( E_F \). Interestingly, and in contrast to the case of Fe|MgO junctions, this is the case also for the BZ center.

It is also interesting to note that the spin-polarized transmission, defined as \( t_k^\uparrow - t_k^\downarrow \), shows that for different pockets in the BZ, the spin of the current-carrying electrons is opposite. For example, for the GPG junction and P configuration the electrons have up spin for the pockets close to the BZ center, while they have down spin for the pockets at the BZ boundary. In contrast, for the AP configuration the pockets at \( k_x = 0 \) have up spins, while the ones at \( k_x = 0 \) have down spins, so that the fourfold rotational symmetry in the \((x,y)\) plane is broken. This is due to the fact that the GPG structure breaks this symmetry in the \((x,y)\) plane, since the Ga-P bonds at the two interfaces are 90° rotated with respect to each other. The imprint of such geometric asymmetry in the transmission indicates a strong contribution of \( d \) orbitals around \( E_F \).

Finally, we look at the Fermi-level PDOS and in particular the spin PDOS (sPDOS), which we define as the difference for spin-up and spin-down PDOS, as a function of the atomic position \( a \) starting from the center of the junction (Fig. 5). sPDOS(\( a \)) at \( E_F \) is staggered on the Mn sites and consistently oppositely polarized to the on-site Mn spin (see Fig. 1). Importantly, there is a notable difference between the two junctions. For both PGP and GPG, the sPDOS(\( a \)) curves for the two P-state partitions and for the AP:(C \rightarrow L) case are identical. However, the remaining different curve AP:(C \rightarrow R) has a cumulative sPDOS with an opposite sign for the GPG

\[^2\text{We approximate the critical current as } I_c = \frac{e}{2}\tau_\pi V_e.\]
cases. The symbol legend is in (d). Spin PDOS is shown, integrated from the center of the junction in all P and AP spin state of each junction. In (c) and (d) the cumulative position in one of the two partitions [(C in the right-hand-side lead between the P and the AP state. Spins swap as the noncompensated spin polarization reverses Fig. 5(d) that the PDOS distributions for majority and minority as described by the Jullière model [17]. In fact, it can be seen in Fig. 5(d) that the PDOS distributions for majority and minority spins swap as the noncompensated spin polarization reverses in the right-hand-side lead between the P and the AP state.

In the SM [7] we provide a detailed analysis of the k⊥-dependent sPDOS around $E_F$, and we show further evidence that, while for the GPG structure the transmission properties are mainly driven by bulklike features, for the PGP they are determined by interface states. The LL and RL interfacial Mn layers (10-Mn in Fig. 3) in the GPG case have large positive $k_\perp$-dependent PDOS, and the spin polarization is very different from the bulk-Mn sPDOS structures in the reciprocal space. For both junctions in the AP state the 10-Mn (RL) shows the exact opposite negative spin polarization (from the P state), and only in the next 11-Mn layer the spin polarization is positive. Evidently, the effective tunneling distance for each spin channel for the bulklike states of GPG is therefore increased for the AP configuration compared to the P one, so a smaller conductance for the AP in this case is expected, manifesting itself in the positive TMR [Fig. 3(f)]. In the PGP case the TMR is governed by the symmetries of the interface states and shows a resonant nature.

In conclusion, we have shown that MTJ stacks made solely of antiferromagnets display staggered spin-transfer torques when the current flows in a direction perpendicular to the plane. This fact is little affected by surface termination and strongly suggests that the AF order parameter can be manipulated by currents. Furthermore, such junctions exhibit pronounced magnetoresistance, which is intrinsic of having a global inversion asymmetry in the stacks. We have deliberately suppressed some of the interface-driven structural inversion asymmetry and compared two junctions which defer by their spacer terminations. We have demonstrated that even under such symmetry enhancement the CuMnAs-based junctions show a significant magnetoresistance effect and that a Ga-Cu termination of the CuMnAs|GaP interface particularly improves the TMR robustness. Our work thus demonstrates that all-antiferromagnetic junctions are both readable and writable with an electrical current, and therefore are interesting candidates as high-frequency, high-density memory elements.

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FIG. 5. (a), (b) Fermi-level spin PDOS as a function of atom position in one of the two partitions [(C → L) or (C → R)] for the P and AP spin state of each junction. In (c) and (d) the cumulative spin PDOS is shown, integrated from the center of the junction in all cases. The symbol legend is in (d).
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