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Large Chiral Orbital Texture and Orbital Edelstein Effect in Co/Al Heterostructure

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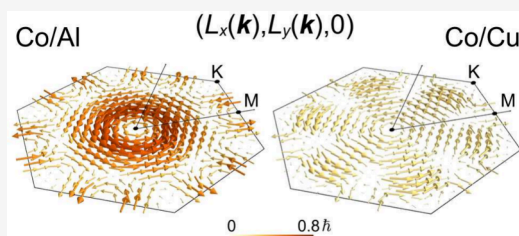
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ABSTRACT: Recent experiments by S. Krishnia et al. [*Nano Lett.* 2023, 23, 6785] reported an unprecedentedly large enhancement of torques upon inserting thin Al layer in Co/Pt heterostructure that suggested the presence of a Rashba-like interaction at the metallic Co/Al interface. Based on first-principles calculations, we reveal the emergence of a large helical orbital texture in reciprocal space at the interfacial Co layer, whose origin is attributed to the orbital Rashba effect due to the formation of the surface states at the Co/Al interface and where spin–orbit coupling is found to produce smaller contributions with a higher-order winding of the orbital moments. Our results unveil that the orbital texture gives rise to a nonequilibrium orbital accumulation producing large current-induced torques, thus providing an essential theoretical background for the experimental data and advancing the use of orbital transport phenomena in all-metallic magnetic systems with light elements.

KEYWORDS: orbitronics, spin–orbit torques, orbital chiral texture, orbital Edelstein effect



Search for efficient ways to control the magnetization in magnetic materials has been one of the central activities in the field of spintronics, which exploits the intrinsic spin of an electron with a focus on providing novel functionalities in electronic devices. In this regard, spin–orbit coupling (SOC) has brought a progressive venue to achieving high-efficiency electrical control of magnetization via spin–orbit torques (SOT),¹ which historically relied on two cornerstone mechanisms. On the one hand, the spin Hall effect in nonmagnetic materials with strong SOC, such as Pt, allows generating spin currents in response to the flowing charge current.^{2–5} On the other hand, spatial inversion symmetry breaking at the interface can give rise to the spin Rashba–Edelstein effect when a nonequilibrium spin accumulation δS is produced by an electric field as a result of the interplay of low dimensionality and SOC.^{6,7} Both the spin currents, when injected into adjacent magnetic layers, and the local spin accumulation induced at the interface of a magnetic heterostructure can exert a SOT on the local magnetic moments M , which is conventionally characterized in terms of the field-like $\tau_{FL} \sim m \times \delta S$ and damping-like $\tau_{DL} \sim m \times (m \times \delta S)$ components with $m = M/|M|$.⁸ The spin Hall effect is considered the primary source of τ_{DL} in metallic systems,^{9,10} while τ_{FL} is predominantly associated with the Rashba–Edelstein effect at the ferromagnet/oxide interfaces.¹¹ In general, both effects act in concert producing SOTs, whose competition governs magnetization dynamics and upon which reversible magnetization switching^{11–14} and domain wall motion^{15–18} can be achieved in a very efficient way.

Over the recent years, there has been a lot of evidence that the spin Hall and Rashba–Edelstein effects may not be the only principal ways to generate SOTs. It was shown theoretically that, in addition to the spin accumulation, a flowing charge current can induce a nonequilibrium orbital accumulation, and, similar to the spin Hall effect, one can realize electrical generation of the transverse orbital currents, or the orbital Hall effect, which is, in many cases, predicted to exceed its spin counterpart.^{19,20} In the same vein, the breaking of spatial inversion symmetry at the interface can result in nontrivial orbital textures in the momentum space regardless of the presence of SOC and the so-called “orbital Rashba effect”^{21–26} which can produce a substantial orbital accumulation under applied electric fields due to the orbital Edelstein effect.^{27,28} Importantly, several studies established that SOTs can be partly mediated by orbital angular momentum and that the injection of orbital currents into a ferromagnet can excite magnetization dynamics.^{29,30} Nowadays, orbitronics is an emerging field of research that aims at exploiting the transport of orbital angular momentum and explores possibilities for generating and manipulating the orbital currents, either alongside or independently of the spin degrees of freedom,

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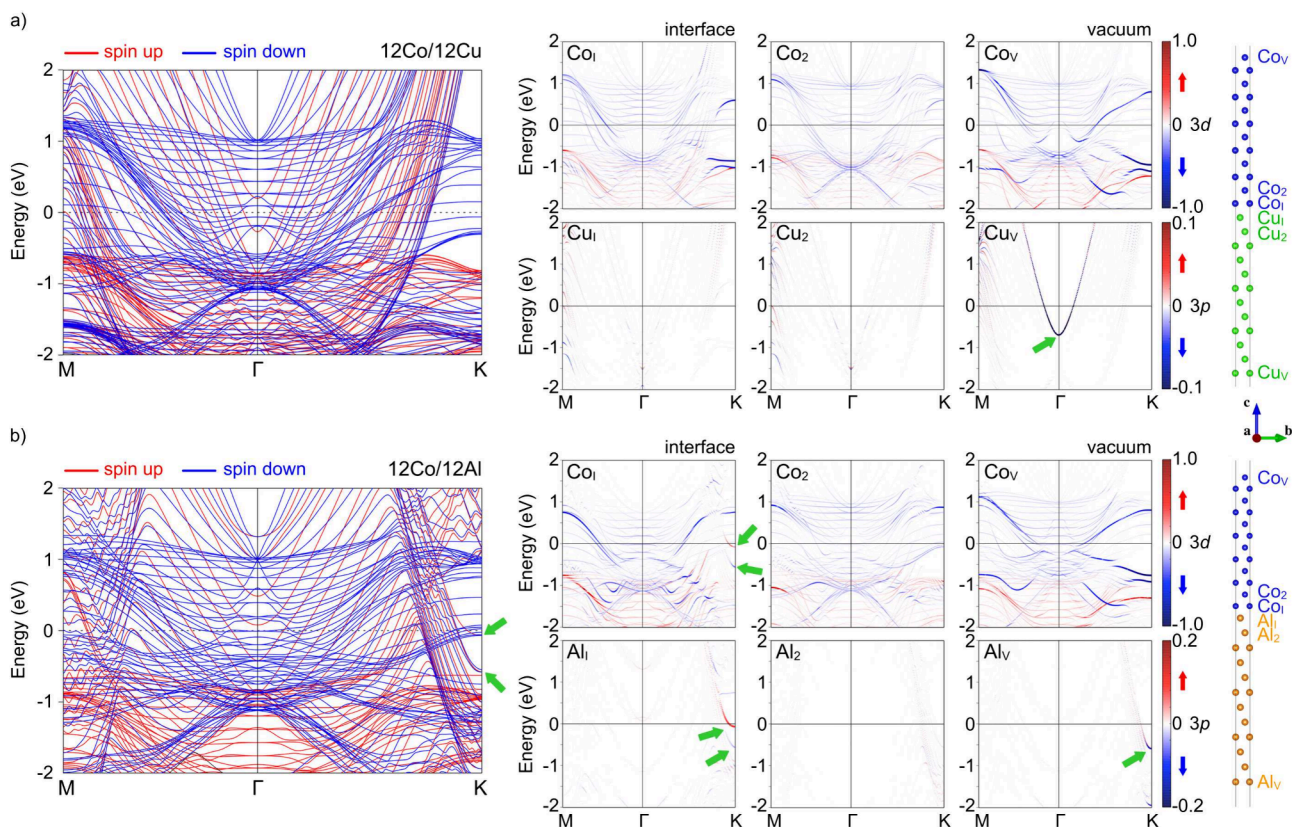


Figure 1. Electronic band structures of (a) 12Co(0001)/12Cu(111) and (b) 12Co(0001)/12Al(111) heterostructures as obtained from GGA calculations without spin–orbit coupling, and layer-resolved projections of the band structure with spin–orbit coupling onto the corresponding atomic orbitals (Cu 3*p*, Al 3*p*, and Co 3*d* orbitals). Green arrows denote the surface states at the interfacial (I) and boundary (V) layers. Red and blue color codes stand for the spin-up and spin-down projections, respectively.

which spurred an ongoing experimental endeavor on direct observation of the orbital transport phenomena.^{31–34} In the context of magnetic torques, recent experimental studies revealed large enhancement of SOTs in thulium iron garnet TmIG/Pt/CuO_x³⁵ and CoFe/Cu/Al₂O₃³⁶ heterostructures which were proposed to be of the orbital origin.

Our recent experiments demonstrated strong enhancement of the current-induced torques in ultrathin Co ferromagnet by insertion of light metal elements.³⁷ In particular, an unprecedentedly large ratio of the field-like and damping-like torques has been observed upon adding thin Al layer to Co/Pt heterostructure. With 3 nm of Al, τ_{FL} and τ_{DL} are increased up to a factor of 11 and 5, respectively, as compared to the same stacking without Al, while similar stackings with Cu inserted instead of Al are found to have negligible effects on the torques. Such giant enhancement of the current-induced torques by introduction of Al layer adjacent to Co and the predominance of the FL torque over the DL torque support the interfacial origin of SOTs and the existence of a large Rashba-type interaction, which is, in turn, not expected for a light-metal interface. Yet, since SOC is small in light elements such as Al, the induced SOTs cannot be directly ascribed to conventional spin Hall and Rashba–Edelstein effects. Despite a number of pioneering studies uncovering the theory of orbital torques, the microscopic origin of enhanced current-induced torques in these systems remains to be understood.

In the present study, we provide a detailed theoretical evidence on the existence of a large chiral orbital texture at the Co/Al interface and the orbital origin of SOTs in Co/Al

heterostructure. We carry out first-principles calculations for Co(0001)/Cu(111) and Co(0001)/Al(111) heterostructures with a single interface and vacuum region by varying the number of constituent layers and considering several possible stackings at the interface. Electronic structure calculations are performed within density functional theory and generalized gradient approximation³⁸ (GGA), as implemented in the Vienna Ab-initio Simulation Package.^{39–41} All calculations consider the ferromagnetic state, with an easy axis perpendicular to the interface in the presence of SOC, and structural optimization is carried out for each considered heterostructure. Further details are given in [Section I of the Supporting Information](#).

The calculated electronic structures of Co/Cu and Co/Al heterostructures shown in [Figure 1](#) suggest that the interfacial Co layers (Co_I) possess several distinct features which are determined by hybridization with the adjacent nonmagnetic layers. In order to understand the essential differences in both interfaces, we can start by analyzing how the interfacial electronic states change in comparison to those of the off-lying layers. The spin nonpolarized surface states are formed at the outmost Cu layer next to the vacuum region (Cu_V in [Figure 1a](#)) which are located at the Γ point of the Brillouin zone and have a predominantly Cu *p_z* orbital character (see [Figures S2 and S3 in the Supporting Information](#)). Similarly, the surface states are realized at the boundary Al layer (Al_V in [Figure 1b](#)) which are, in contrast, located at the *K* point and formed by the Al *p_x* and *p_y* orbitals (see [Figures S4 and S5 in the Supporting Information](#)). At the interface, the hybridization

primarily occurs between the Al/Cu p and Co d orbitals, being more pronounced in the vicinity of the K point at the Co/Al interface due to the presence of the surface states. Indeed, while the hybridization clearly modifies the states at the interfacial layers in both systems, one can see that the difference between the interfacial and boundary Co $3d$ states (Co_1 and Co_V) is more striking in the case of Co/Al heterostructure. Namely, the surface states become spin-polarized at the Co/Al interface due to the proximity effect (Al_1 and Co_1 in Figure 1b), but vanish at the interfacial Cu layer (Cu_1 in Figure 1a). Moreover, as a result of the interfacial hybridization, both spin and orbital magnetic moments of Co presented in Figure 2 are relatively decreased at the Co/Al interface, as opposed to the Co/Cu interface, where neither of the magnetic moments reveals noticeable changes across the heterostructure.

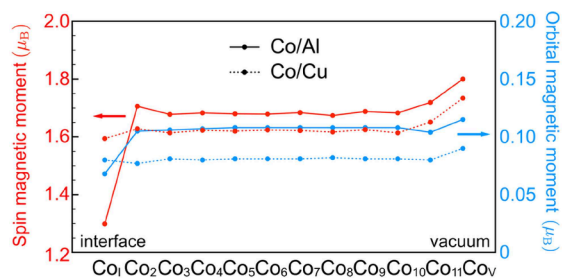


Figure 2. Spin and orbital magnetic moments at Co layers in $12\text{Co}(0001)/12\text{Cu}(111)$ and $12\text{Co}(0001)/12\text{Al}(111)$ heterostructures as obtained from GGA calculations with spin–orbit coupling. Only z components are shown, x and y components are zero at each layer.

Drastic changes in electronic and magnetic properties at the Co/Al and Co/Cu interfaces can be observed by calculating the orbital and spin profiles in reciprocal space, $L(\mathbf{k}) = \sum_n L_n(\mathbf{k})f_{nk}$ and $S(\mathbf{k}) = \sum_n S_n(\mathbf{k})f_{nk}$ respectively, where f_{nk} is the Fermi–Dirac occupation function with respect to the Fermi level, and n runs over all bands. Here, $L_n(\mathbf{k}) = \langle u_{nk} | \hat{L} | u_{nk} \rangle$ and $S_n(\mathbf{k}) = \langle u_{nk} | \hat{S} | u_{nk} \rangle$ are the matrix elements of the orbital and spin angular momentum operators calculated by projecting the Bloch wave functions $|u_{nk}\rangle = \sum_{\mu\sigma} a_{\mu nk}^{\sigma} |\mu\sigma\rangle$ onto atomic orbitals $|\mu\sigma\rangle$, with μ and σ encoding orbital and spin indices, respectively. From the profiles shown in Figure 3, one can see that both $S(\mathbf{k})$ and $L(\mathbf{k})$ exhibit a 3-fold rotational texture, in agreement with the C_{3v} symmetry of the constructed heterostructures. The alternating pattern of $L_z(\mathbf{k})$ coming from nonzero matrix elements $\langle d_{yz} | \hat{L}_z | d_{zx} \rangle = i$ and $\langle d_{xy} | \hat{L}_z | d_{x^2-y^2} \rangle = 2i$ is found to be strongly suppressed at the interfaces as compared to the interior layers. With the changes being seemingly identical at both interfaces, the average value of $L_z(\mathbf{k})$ over the Brillouin zone yields a decreased orbital moment for the Co/Al interface, in agreement with Figure 2. More strikingly, the hybridization at the Co/Al interface turns out to give rise to an exceptionally large orbital texture with an in-plane helical locking at the interfacial Co layer, as opposed to the Co/Cu interface where the in-plane orbital texture is much less pronounced. Following the orbital character of the states hybridized at the interface, the largest contribution to the chiral orbital texture is found to arise from nonzero matrix elements $\langle d_{yz} | \hat{L}_x | d_{yz} \rangle = \sqrt{3}i$ and $\langle d_{yz} | \hat{L}_y | d_{zx} \rangle = -\sqrt{3}i$. Given that the hybridization occurs between the Al p_x and p_y and Co d_{z^2} , d_{zx} and d_{yz} orbitals, the emergence of the chiral orbital texture at the interfacial Co layer can be attributed to the so-called orbital Rashba effect^{21–24,26} as a result of peculiar hybridization with the surface states at the interface. It is worth noting that

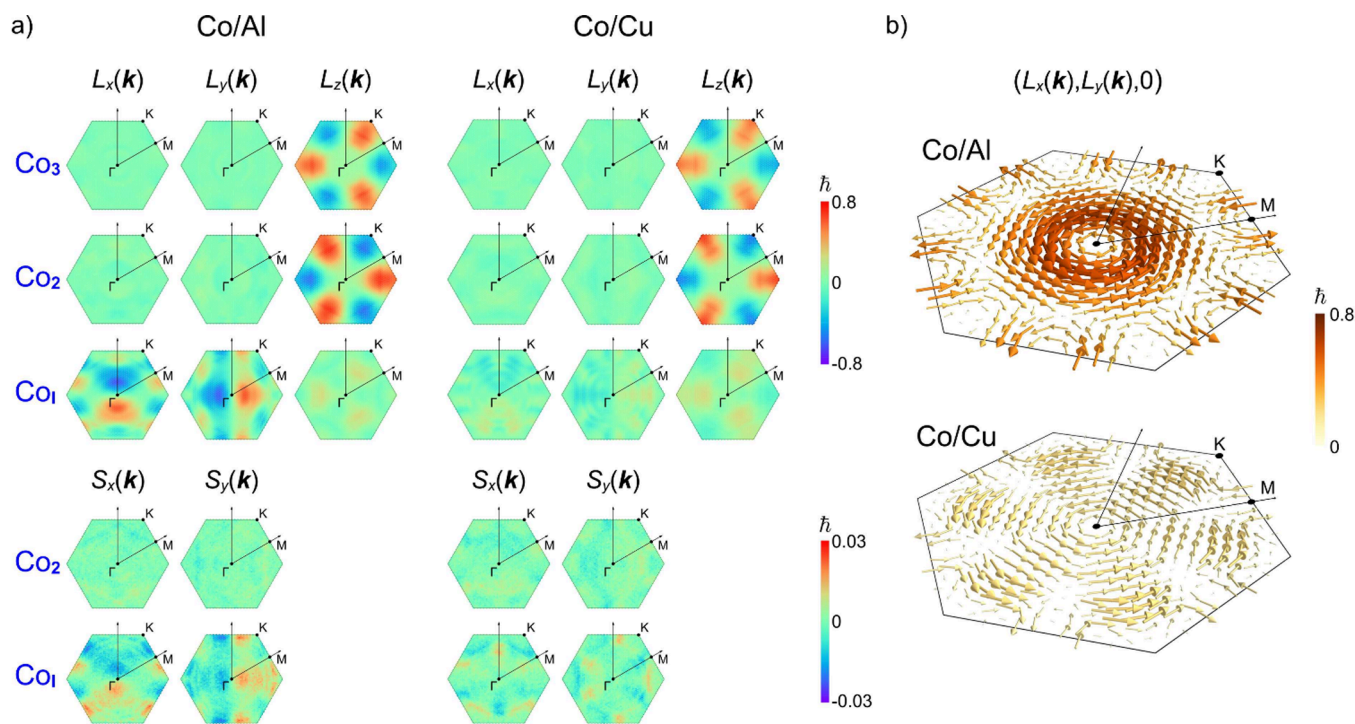


Figure 3. (a) Layer-resolved orbital and spin profiles in the Brillouin zone calculated for $12\text{Co}(0001)/12\text{Al}(111)$ and $12\text{Co}(0001)/12\text{Cu}(111)$ heterostructures with spin–orbit coupling. $L(\mathbf{k})$'s integrated over the Brillouin zone correspond to the orbital magnetic moments presented in Figure 2. (b) In-plane orbital textures at the interfacial Co layer. Arrows for the Co/Cu interface are magnified by a factor of 2 for clarity.

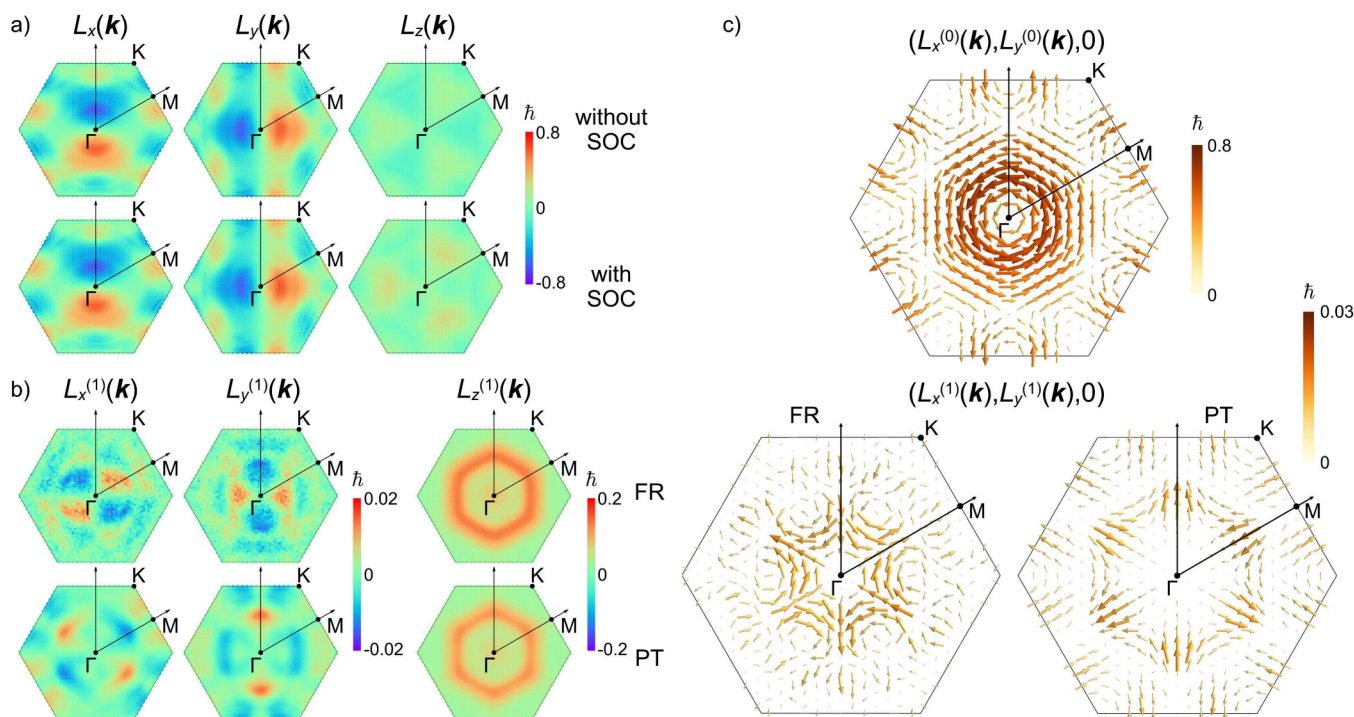


Figure 4. (a) Orbital profiles $L(\mathbf{k})$ at the interfacial Co layer in 12Co(0001)/12Al(111) heterostructure as obtained from electronic structure calculations with and without spin–orbit coupling. (b) Orbital profile $L^{(1)}(\mathbf{k})$ induced by spin–orbit coupling as obtained from fully relativistic electronic structure calculations (FR) and perturbation theory (PT). (c) In-plane orbital textures $L^{(0)}(\mathbf{k})$ and $L^{(1)}(\mathbf{k})$.

the chiral orbital texture at the Co/Al interface does not change qualitatively upon including the on-site Coulomb repulsion in the Co 3d orbitals, which changes the splitting between the fully occupied spin-up and partially occupied spin-down Co 3d states (see Figures S6–S13 with the results of GGA+U calculations in the Supporting Information).^{42–45} Neither does it change upon considering different stackings at the interface or changing the number of layers in the heterostructure (see Figure S14 in the Supporting Information), thus implying that the emergence of the chiral orbital texture can be regarded as a robust feature of the Co/Al interface due to the formation of the surface states. Finally, we note that the transverse spin profile $S_x(\mathbf{k})$ and $S_y(\mathbf{k})$ is found to have a similar chiral pattern at the interface of Co/Al heterostructure but is much smaller in magnitude (see also Figure S13 in the Supporting Information).

As follows from Figure 4a, the in-plane orbital texture at the Co/Al interface is preserved without SOC, as opposed to the transverse spin texture which is identically zero in the absence of relativistic effects. Without SOC, $L(\mathbf{k}) = -L(-\mathbf{k})$ holds true owing to time-reversal symmetry yielding the net orbital moment to be identically zero, when integrated over the Brillouin zone. In the presence of SOC, the magnetization direction is fixed along the easy axis, and time-reversal symmetry is broken leading to $L(\mathbf{k}) \neq -L(-\mathbf{k})$ with a nonzero net orbital moment. To gain further insight into the origin of the chiral orbital texture, it is expedient to decompose the orbital moment as a sum of two contributions $L(\mathbf{k}) = L^{(0)}(\mathbf{k}) + L^{(1)}(\mathbf{k})$, where the first term $L^{(0)}(\mathbf{k}) = 1/2(L(\mathbf{k}) - L(-\mathbf{k}))$ represents the time-reversal symmetric contribution, while the second one $L^{(1)}(\mathbf{k}) = 1/2(L(\mathbf{k}) + L(-\mathbf{k}))$ can be identified with a nonvanishing net orbital moment, with respect to the magnetization in the presence of SOC. Thus, $L(\mathbf{k}) = L^{(0)}(\mathbf{k})$ and $L^{(1)}(\mathbf{k}) = 0$ in the absence of SOC, and

SOC can generally contribute to both terms. From a practical point of view, one can find $L^{(1)}(\mathbf{k})$ either directly from fully relativistic electronic structure calculations including SOC using the definition above or by treating SOC within perturbation theory starting from the electronic structure calculated without SOC.^{46–48} For the latter, $L^{(1)}(\mathbf{k})$ can be derived by decomposing the Bloch wave functions over the basis of cubic harmonics that yields to first order in SOC:

$$L^{(1)}(\mathbf{k}) = -\xi_{Re} \sum_{\nu\mu\mu'\nu'} \langle \nu | \hat{L} | \nu' \rangle \langle \mu' | \hat{L} \cdot \mathbf{m} | \mu \rangle (A_{\nu\mu\mu'\nu'}^{\uparrow\uparrow}(\mathbf{k}) - A_{\nu\mu\mu'\nu'}^{\downarrow\downarrow}(\mathbf{k})) \quad (1)$$

where $\xi = 69.4$ meV is the SOC constant adopted for Co atoms,^{49–51} and $A_{\nu\mu\mu'\nu'}^{\sigma\sigma'}(\mathbf{k})$ is the generalized susceptibility of linear response theory with μ, μ', ν, ν' and σ, σ' being orbital and spin indices, respectively (see Section II in the Supporting Information). As one can see in Figure 4b for the out-of-plane direction of magnetization $\mathbf{m} \parallel \mathbf{e}_z$, the inclusion of SOC results in a symmetric pancake-like profile for $L_z^{(1)}(\mathbf{k})$ giving the net orbital moment along the magnetization. In addition, the in-plane profile of $L^{(1)}(\mathbf{k})$ shown in Figure 4c has a higher-order winding of the orbital moment obeying the C_{3v} symmetry and can be regarded as the SOC driven contribution to the orbital Rashba effect, similar to the spin Rashba effect.⁵² Importantly, the in-plane texture $L^{(0)}(\mathbf{k})$ reveals only minor changes upon including SOC, and $L^{(1)}(\mathbf{k})$ arising from SOC is found to be more than an order of magnitude smaller than $L^{(0)}(\mathbf{k})$, thus implying that the emergence of the chiral orbital texture is essentially determined by the hybridization at the interface.

The results of electronic structure calculations demonstrate that the Co/Al interface features a large in-plane chiral orbital texture. While both $L_x(\mathbf{k})$ and $L_y(\mathbf{k})$ cancel out in equilibrium for $\mathbf{m} \parallel \mathbf{e}_z$, an applied in-plane electric field can induce a finite orbital angular momentum, giving rise to the orbital Edelstein

effect.^{27,28} The current induced orbital accumulation δL can be determined as a linear response to an electric field E by using Kubo theory as $\delta L_\alpha = \chi_{\alpha\beta}^L E_\beta$ where summation over repeated indices is implied ($\alpha, \beta = x, y, z$). Starting from the one-particle picture $\hat{H}_k u_{nk}(\mathbf{r}) = \varepsilon_{nk} u_{nk}(\mathbf{r})$, where \hat{H}_k is the Kohn–Sham Hamiltonian, and $u_{nk}(\mathbf{r})$ is the Bloch wave function for band n at wavevector \mathbf{k} and energy ε_{nk} , the rank-2 orbital magneto-electric susceptibility tensor $\chi_{\alpha\beta}^L$ can be written as a sum of two contributions:^{53,54}

$$\begin{aligned} \delta L_\alpha^{\text{intra}} &= \chi_{\alpha\beta}^{L,\text{intra}} E_\beta \\ &= -eE\tau \sum_{nk} \frac{\partial f_{nk}}{\partial \varepsilon_{nk}} \langle u_{nk} | \hat{L}_\alpha | u_{nk} \rangle \langle u_{nk} | \hat{v}_{\beta,k} | u_{nk} \rangle \end{aligned} \quad (2)$$

$$\begin{aligned} \delta L_\alpha^{\text{inter}} &= \chi_{\alpha\beta}^{L,\text{inter}} E_\beta \\ &= ie\hbar E \sum_{n \neq m, k} \frac{(f_{nk} - f_{mk}) \langle u_{mk} | \hat{L}_\alpha | u_{nk} \rangle \langle u_{nk} | \hat{v}_{\beta,k} | u_{mk} \rangle}{(\varepsilon_{nk} - \varepsilon_{mk})(\varepsilon_{nk} - \varepsilon_{mk} - i\hbar\tau^{-1})} \end{aligned} \quad (3)$$

where e (<0) is the electron charge, $\hat{v}_k = \frac{1}{\hbar} \partial_k \hat{H}_k$ is the velocity operator, and τ is the characteristic relaxation time defining the broadening of the electronic spectrum. The first and second terms correspond to the intraband contribution of the states at the Fermi surface and the interband transitions coming from the Fermi sea, respectively, summing up to $\chi_{\alpha\beta}^L = \chi_{\alpha\beta}^{L,\text{intra}} + \chi_{\alpha\beta}^{L,\text{inter}}$. In magnetic systems, the susceptibility tensor can be further decomposed into time-reversal-even and time-reversal-odd components as $\chi_{\alpha\beta}^L(\mathbf{m}) = \chi_{\alpha\beta}^{\text{even}}(\mathbf{m}) + \chi_{\alpha\beta}^{\text{odd}}(\mathbf{m})$, with $\chi_{\alpha\beta}^{\text{even}}(\mathbf{m}) = 1/2(\chi_{\alpha\beta}^L(\mathbf{m}) + \chi_{\alpha\beta}^L(-\mathbf{m}))$ and $\chi_{\alpha\beta}^{\text{odd}}(\mathbf{m}) = 1/2(\chi_{\alpha\beta}^L(\mathbf{m}) - \chi_{\alpha\beta}^L(-\mathbf{m}))$. Taking the out-of-plane direction of \mathbf{m} and the symmetry of Co/Al heterostructures by construction as the C_{3v} group, one can show that the only nonzero components of $\chi_{\alpha\beta}^L(\mathbf{m})$ are the off-diagonal $\chi_{xy}^{\text{even}}(\mathbf{m}) = -\chi_{yx}^{\text{even}}(\mathbf{m})$ and diagonal $\chi_{xx}^{\text{odd}}(\mathbf{m}) = \chi_{yy}^{\text{odd}}(\mathbf{m}) \neq \chi_{zz}^{\text{odd}}(\mathbf{m})$ susceptibilities (see Section IIIa in the Supporting Information).^{55,56} Following the symmetry analysis for the in-plane orbital texture $L(\mathbf{k})$, it is straightforward to note that $L^{(0)}(\mathbf{k})$ and $L^{(1)}(\mathbf{k})$ determine $\chi_{xy}^{\text{even}}(\mathbf{m})$ and $\chi_{xx}^{\text{odd}}(\mathbf{m})$, respectively. Since $L^{(1)}(\mathbf{k})$ is much smaller than $L^{(0)}(\mathbf{k})$, the off-diagonal susceptibility $\chi_{xy}^{\text{even}}(\mathbf{m})$ originating from the chiral orbital texture $L^{(0)}(\mathbf{k})$ can be considered to generate the leading nonequilibrium orbital response at the Co/Al interface (see Section III d in the Supporting Information). Calculations of the orbital susceptibility tensor are performed using the Wannier interpolation^{57,58} of the electronic structure along the lines with previous studies on the anomalous and spin Hall susceptibilities (see Section III b in the Supporting Information).^{59–61} Given the smallness of $L^{(1)}(\mathbf{k})$ and that $L^{(0)}(\mathbf{k})$ does not depend on the magnetization to first order in SOC, χ_{xy}^L can be calculated without SOC. The results shown in Figure 5 illustrate that the orbital magnetoelectric susceptibility at the interfacial Co layer stands out in magnitude in comparison with the interior Co layers. The diagonal components χ_{xx}^{even} are identically zero in agreement with the symmetry consideration.

The induced orbital accumulation δL couples to the spin accumulation δS by means of SOC and can exert a torque $\boldsymbol{\tau} = \mathbf{M} \times \delta \mathbf{B}_{\text{xc}}$ on the magnetization, where $\delta \mathbf{B}_{\text{xc}} \sim \delta S$ is a change in the effective exchange-correlation magnetic field caused by the nonequilibrium spin accumulation. Given the in-plane electric field E and the normal direction e_z , the spin accumulation δS

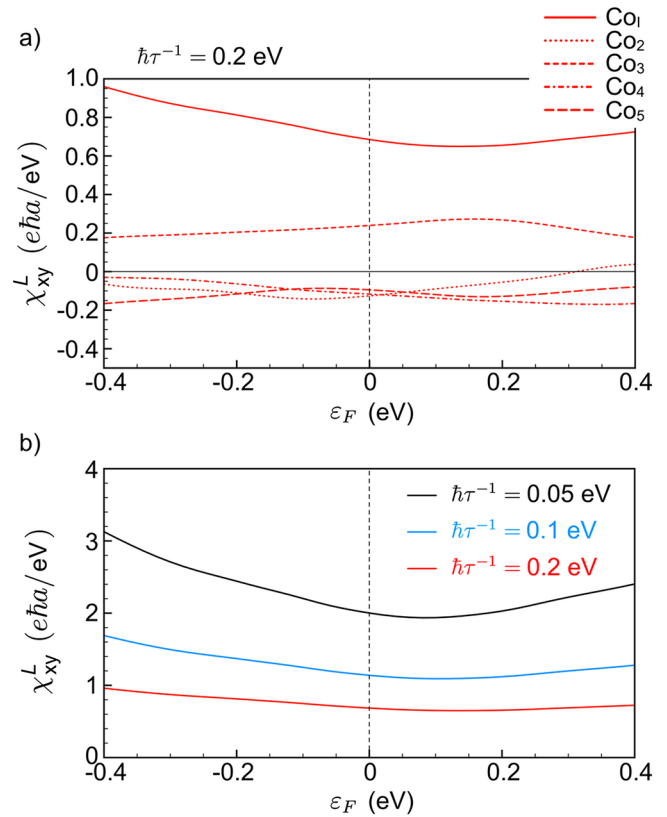


Figure 5. (a) Off-diagonal orbital magnetoelectric susceptibility χ_{xy}^L calculated for 8Co(0001)/6Al(111) heterostructure without spin-orbit coupling as a function of the Fermi level ε_F . (b) χ_{xy}^L at the interfacial Co layer calculated for different relaxation times. Here, a is the optimized lattice constant (~ 2.63 Å for 8Co(0001)/6Al(111) heterostructure). Calculations are performed on a $100 \times 100 \times 1$ k -point mesh with the temperature factor $k_B T = 0.1$ eV.

can be decomposed into the E -transverse $\sim E \times e_z$ and M -transverse $\sim \mathbf{m} \times (E \times e_z)$ components, where the former is time-reversal even and does not depend on the magnetization direction, while the latter depends on the orientation of \mathbf{m} with respect to E and e_z . Thus, it follows that the field-like $\boldsymbol{\tau}_{\text{FL}} \sim \mathbf{m} \times (E \times e_z)$ and the damping-like $\boldsymbol{\tau}_{\text{DL}} \sim \mathbf{m} \times (\mathbf{m} \times (E \times e_z))$ torques can be expressed through the off-diagonal $\chi_{xy}^{\text{even}}(\mathbf{m})$ and diagonal $\chi_{xx}^{\text{odd}}(\mathbf{m})$ components, respectively. Using the results of linear response theory, one can estimate the effective magnetic field producing $\boldsymbol{\tau}_{\text{FL}}$ as $B_{\text{FL}} = \xi \chi_{xy}^L E / (M_s d_F)$ (see Section III c of the Supporting Information) that for the thickness $d_F \approx 10^{-9}$ m, $E \approx 2.5 \times 10^4$ V/m (for the spin current density $J^S \approx 10^{11}$ A/m² in the experimental results), saturation magnetization $M_s \approx 1.4 \times 10^6$ A/m, $\xi \approx 10^{-20}$ J, and $\chi_{xy}^L \approx 2.0 \times 10^{10} \hbar$ m/V (for $\hbar\tau^{-1} = 0.05$ eV and $\varepsilon_F = 0$) gives $B_{\text{FL}} = 3.6$ mT, of comparable magnitude with the increase of B_{FL} by ~ 7 mT, with respect to its value ~ 0.6 mT before insertion of Al.³⁷ With the diagonal components $\chi_{\alpha\alpha}^L$ being an order of magnitude smaller, the associated contribution to the damping-like torque can be regarded small compared to $\boldsymbol{\tau}_{\text{FL}}$. That being said, $\boldsymbol{\tau}_{\text{DL}}$ is also likely to originate either from the diffusion of the orbital accumulation into the interior layers, which is further transferred to the magnetization by SOC-induced orbital precession, or indirectly, by conversion to the spin accumulation and subsequent transfer to the magnetization by spin precession. This generation of $\boldsymbol{\tau}_{\text{DL}}$ by out-of-equilibrium processes, not calculated here, is expected to be

smaller than the field-like torque produced by SOC directly from the interfacial orbital accumulation, the predominance of which is seen in the experiments. Our analysis is also in good agreement with micromagnetic estimates suggesting that large spin accumulation induced by a Rashba-like interaction at the interface is required to fit the experimental data.³⁷

In conclusion, the results of first-principles calculations demonstrate that the Co/Al interface features a large orbital texture with the in-plane helical locking of the orbital moment in reciprocal space, which is found to be much smaller at the Co/Cu interface. The origin of the chiral orbital texture is attributed to the orbital Rashba effect due to the formation of the surface states at the interface with smaller higher-order contributions coming from SOC. Our calculations unveil that the orbital texture is responsible for the conversion effects in response to an applied electric current that produce large field-like torques at the Co/Al interface, thus providing a rigorous theoretical interpretation for recent experiments³⁷ and advancing our understanding of transport phenomena in all-metallic systems with light elements for spinorbitronic-based technologies.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.nanolett.4c01607>.

Computational details of electronic structure calculations; perturbation theory for the orbital magnetic moment; calculations of the orbital magnetoelectric tensor (PDF)

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Notes

The authors declare no competing financial interest.

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