

Pure Spin Current Injection in Hydrogenated Graphene Structures

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We present a theoretical study of spin-velocity injection with linearly polarized light of two 50% hydrogenated noncentrosymmetric graphene structures: Alt and Up. We analyzed the cases when the spin is polarized perpendicularly to the surface of the structures, in the z direction, and when the spin moves along the fixed x and y directions. The results are calculated in a full electronic band structure scheme within DFT in the LDA approximations showing an anisotropic behavior. We obtained maximum absolute values of $\mathcal{V}_{\sigma z}(\omega, \alpha) = 668.0 \text{ Km/s}$ for the Up structure and $\mathcal{V}^y(\omega, \alpha) = 905.6 \text{ Km/s}$ for the Alt structure being both structures excellent candidates for spintronics applications.

I. INTRODUCTION

sec:introduction

Spintronics is an emerging research field of electronics in which the manipulation and transport of spin of electrons in a solid state media plays the determining role adding a new degree of freedom to the conventional charge manipulation.^{1,2} At present there is an increasing interest in attain the same level of control over the transport of spin at micro or nano scales as has been done for the flow of charge in typical electronic devices.³ Some semiconductor spintronics devices have been proposed^{4–7} and some of them require spin polarized electrical current⁸ or pure spin current (PSC). One of the difficulties to achieve the development of spin current and PSC semiconductor devices is the fact that the spin relaxation time in a semiconducting media is short disabling the spin transport and then resulting in a no observable spin current.⁹ In PSCs there is no net motion of charge; spin-up electrons move in a given direction while spin-down electrons travel in the opposite one. This effect can result from one photon absorption of linearly polarized light by a semiconductor, with filled valence bands and empty conduction bands, illuminated by light with photon energy larger than the energy gap. For instance, this phenomena can result from spin injection,¹⁰ Hall

Effects,¹¹ interference of two optical beams,^{12,13} or one photon absorption of linearly polarized light¹⁴ and has been observed in gallium arsenide (GaAs),^{15,16} aluminum-gallium arsenide (AlGaAs),¹⁶ and Co₂FeSi.¹⁷

Graphene, an allotrope of carbon with hexagonal 2D lattice structure presents properties like fractional quantum Hall effect at room temperature, excellent thermal transport properties, excellent conductivity¹⁸ and strength^{19–22} being then a perfect platform to be used in two-dimensions electronic systems; however most electronic applications are disabled by the absence of a semiconducting gap. Recent studies demonstrate that the band gap of graphene can be opened by applying an electric field,²³ reducing the surface area,²⁴ or applying uniaxial strain.²⁵ Another possibility to open the gap is by doping; this has been successfully achieved using nitrogen,²⁶ boron-nitrogen,²⁷ silicon,²⁸ noble-metals,²⁹ and hydrogen.^{30–32} Depending on the percentage of hydrogenation and spatial configurations of hydrogen-carbon bonds, hydrogenated graphene can result in different spatial configurations. In this paper we present two 50% hydrogenated graphene noncentrosymmetric structures both presenting a discernible band gap: the Up structure, shown in Fig. 1, has hydrogen atoms bonded to the carbon layer only

in the upper side of the structure while the Alt structure, shown in Fig. 2, has hydrogen alternating in the upper and bottom sides of the carbon slab.³³

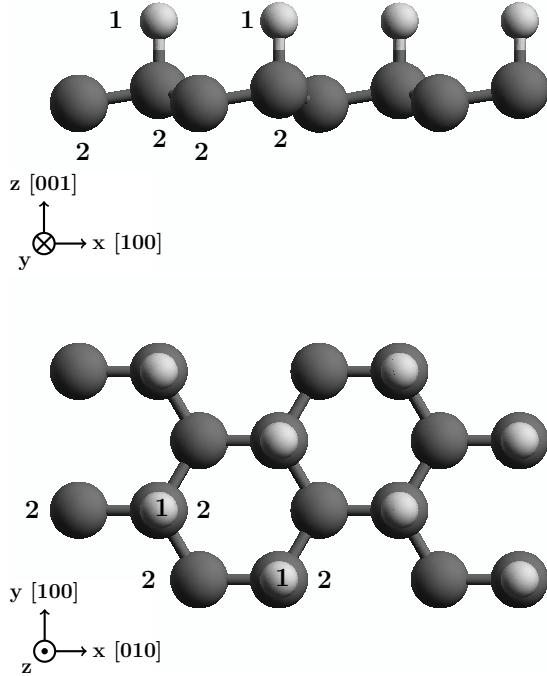


FIG. 1. Side (top panel) and top (bottom panel) views of the Up structure along with the Cartesian xyz directions. The dark (light) spheres are the C (H) atoms, labeled 1 (2).

`fig:up-struc`

Using those structures we address a theoretical study of the spin velocity injection (SVI) by one-photon absorption of linearly polarized light. Because we have 2D structures we made the analysis for two cases. The first is fixing the spin of the electrons along the z Cartesian direction with the velocity directed on the surface of the structure in the xy plane. The second is fixing the spin velocity in the x or y direction and the spin directed in xyz . The SVI is an optical effect that quantifies the velocity at which a PSC moves along the Cartesian direction a with the spin of electron polarized along the Cartesian direction b . One photon absorption of linearly polarized light can promote an even distribution of electrons in \mathbf{k} space regardless the symme-

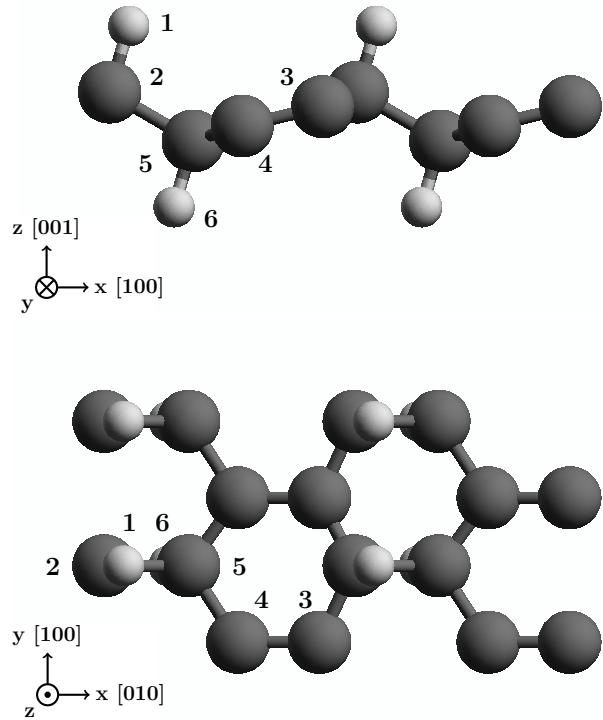


FIG. 2. Side (top panel) and top (bottom panel) views of the Alt structure along with the Cartesian xyz directions. The dark (light) spheres are the C (H) atoms, labeled 1 (2).

`fig:alt-struc`

try of the material resulting in a null electrical current.¹⁴ Then, the electrons excited to the conduction bands at opposite \mathbf{k} points will result in opposite spin polarizations producing no net spin injection.¹⁴ If the crystalline structure of the material is noncentrosymmetric the spin polarization injected at a given \mathbf{k} point not necessarily vanishes,^{34,35} and then, since the velocities of electrons at opposite \mathbf{k} points are opposite, a PSC will be produced. Since the structures presented here are noncentrosymmetric, they are good candidates in which this effect can be induced.

This paper is organized as follows. In Section II we present the theory and formulas that describe PSC and SVI. In Section III we describe the details of calculations and the corresponding SVI spectra for the Up and Alt structures. Finally, we present our conclusions in Section IV.

II. THEORY

sec:theory

In this section, we report a summary of the theory involved in the calculation of the spin velocity injection (SVI) resulting from the pure spin current (PSC).

The operator that describes the electronic SVI is written as

$$\hat{K}^{ab} = \frac{1}{2} (\hat{v}^a \hat{S}^b + \hat{S}^b \hat{v}^a), \quad z(1)$$

where $\hat{\mathbf{v}} = [\hat{\mathbf{r}}, \hat{H}_0]/i\hbar$ is the velocity operator, with $\hat{\mathbf{r}}$ the position operator, \hat{H}_0 the unperturbed ground state Hamiltonian, and the Roman superscripts indicate Cartesian coordinates. To obtain the expectation value of \hat{K}^{ab} , we use the length gauge for the perturbing Hamiltonian, written as

$$\hat{H}_p = -e\hat{\mathbf{r}} \cdot \mathbf{E}(t), \quad z(2)$$

where the electric field of the applied laser is given by

$$\mathbf{E}(t) = \mathbf{E}(\omega)e^{-i\omega t} + \mathbf{E}^*(\omega)e^{i\omega t}. \quad z(3)$$

In order to calculate the response of the system to $\mathbf{E}(t)$, one needs to take into account the excited coherent superposition of the spin-split conduction bands inherent to the noncentrosymmetric semiconductors considered in this work. To include the coherences, we follow Ref. 36 and use a multiple scale approach that solves the equation of motion for the single particle density matrix $\rho_{mn}(\mathbf{k}; t)$, leading to

$$\begin{aligned} \frac{\partial \rho_{cc'}(\mathbf{k})}{\partial t} &= \frac{e^2 E^a(\omega) E^{b*}(\omega)}{i\hbar^2} \sum_v r_{cv}^a(\mathbf{k}) r_{vc'}^b(\mathbf{k}) \\ &\times \left(\frac{1}{\omega - \omega_{c'v}(\mathbf{k}) - i\epsilon} - \frac{1}{\omega - \omega_{cv}(\mathbf{k}) + i\epsilon} \right), \quad z(4) \end{aligned}$$

where we assumed that the conduction bands c and c' are quasidegenerate states and we take $\epsilon \rightarrow 0$ at the end of the calculation. The spin-splitting of the valence (v) bands is very small, and is neglected throughout this work.[?] The matrix elements of any operator \mathcal{O} are given by $\mathcal{O}_{nm}(\mathbf{k}) = \langle n\mathbf{k} | \hat{\mathcal{O}} | m\mathbf{k} \rangle$, where $H_0|n\mathbf{k}\rangle = \hbar\omega_n(\mathbf{k})|n\mathbf{k}\rangle$ with $\hbar\omega_n(\mathbf{k})$ the energy of the electronic band n at point \mathbf{k} in the irreducible Brillouin zone (IBZ), $|n\mathbf{k}\rangle$ is the Bloch state, and

$\omega_{nm}(\mathbf{k}) = \omega_n(\mathbf{k}) - \omega_m(\mathbf{k})$. Using $\mathcal{O} = \text{Tr}(\hat{\rho}\hat{\mathcal{O}})$ for the expectation value of an observable \mathcal{O} , where Tr denotes the trace, we obtain

$$\mathcal{O} = \int \frac{d^3k}{8\pi^3} \sum_{cc'} \rho_{cc'}(\mathbf{k}) \mathcal{O}_{c'c}(\mathbf{k}), \quad z(5)$$

where we used the closure relationship $\sum_n |n\mathbf{k}\rangle \langle n\mathbf{k}| = 1$, where $n = v, c$, and the fact that $\rho_{vn}(\mathbf{k}) = \rho_{nv}(\mathbf{k}) = 0$ for $n = c, c'$. Therefore, using Eqs. (4) and (5), the rate of change of \mathcal{O} , $\dot{\mathcal{O}} = \text{Tr} \left(\frac{\partial \hat{\rho}}{\partial t} \hat{\mathcal{O}} \right)$, is given by

$$\begin{aligned} \dot{\mathcal{O}} &= \frac{e^2}{i\hbar^2} \int \frac{d^3k}{8\pi^3} \sum'_{cc'} \mathcal{O}_{c'c}(\mathbf{k}) r_{cv}^a(\mathbf{k}) r_{vc'}^b(\mathbf{k}) \times \\ &\left(\frac{1}{\omega - \omega_{c'v}(\mathbf{k}) - i\epsilon} - \frac{1}{\omega - \omega_{cv}(\mathbf{k}) + i\epsilon} \right) E^a(\omega) E^{b*}(\omega). \quad z(6) \end{aligned}$$

Replacing $\hat{\mathcal{O}} \rightarrow \hat{K}^{ab}$, in above expression, one can show that

$$\dot{K}^{ab}(\omega) = \mu^{abcd}(\omega) E^c(\omega) E^{d*}(\omega), \quad \text{eq:dotk} \quad z(7)$$

where repeated cartesian are summed, and

$$\begin{aligned} \mu^{abcd}(\omega) &= \frac{\pi e^2}{\hbar^2} \int \frac{d^3k}{8\pi^3} \sum'_{vc'} \delta(\omega - \omega_{cv}(\mathbf{k})) \\ &\times \text{Re} \left[K_{cc'}^{ab}(\mathbf{k}) \left(r_{vc'}^c(\mathbf{k}) r_{cv}^d(\mathbf{k}) + (c \leftrightarrow d) \right) \right], \quad \text{eq:mu} \quad z(8) \end{aligned}$$

is the pseudotensor that describes the rate of change of the PSC process in semiconductors. To derive above we used $K_{nm}^{ab}(-\mathbf{k}) = K_{nm}^{ab*}(\mathbf{k})$, that follows from time-reversal invariance. The prime ' in the sum means that c and c' are quasi degenerate states and the sum only covers these states. Since $\mu^{abcd}(\omega)$ is real we have that $\mu^{abcd}(\omega) = \mu^{abdc}(\omega)$. We remark that Eq. (8) is the same as Eq. (3) of Bhat et al.¹⁴ obtained by using the semiconductor optical Bloch equations. Using the closure relation,

$$K_{cc'}^{ab}(\mathbf{k}) = \frac{1}{2} \sum_{l=v,c} \left(v_{cl}^a(\mathbf{k}) S_{lc'}^b(\mathbf{k}) + S_{cl}^b(\mathbf{k}) v_{lc'}^a(\mathbf{k}) \right). \quad \text{eq:velspimatelem} \quad z(9)$$

Now, we define the spin velocity injection (SVI) as

$$\mathcal{V}^{ab}(\omega) \equiv \frac{\dot{K}^{ab}(\omega)}{(\hbar/2)\dot{n}(\omega)}, \quad \text{eq:vab-w} \quad z(10)$$

that gives the velocity, along the direction a, at which the spin moves polarized along the direction b. The carrier injection rate $\dot{n}(\omega)$ is written as,³⁶

$$\dot{n}(\omega) = \xi^{ab}(\omega) E^c(\omega) E^{d*}(\omega), \quad \text{eq:dotn} \quad (11)$$

where the tensor

$$\begin{aligned} \xi^{ab}(\omega) &= \frac{2\pi e^2}{\hbar^2} \int \frac{d^3 k}{8\pi^3} \\ &\times \sum_{vc} r_{vc'}^a(\mathbf{k}) r_{cv}^b(\mathbf{k}) \delta(\omega - \omega_{cv}(\mathbf{k})), \end{aligned}$$

is related to the imaginary part of the linear optical response tensor by $\text{Im}[\epsilon^{ab}(\omega)] = 2\pi\epsilon_0\hbar\xi^{ab}(\omega)$.

The function $\mathcal{V}^{ab}(\omega)$ allow us to quantify two very important aspects of PSC. On one hand, we can fix the spin direction along b, and calculate the resulting electron velocity. On the other hand, we can fix de velocity of the electron along b, and study the resulting direction along which the spin is polarized. To this end, the added advantage of 2D structures, besides choosing them noncentrosymmetric, is that we can use an incoming linearly polarized beam of light at normal incidence, and use the direction of the polarized electric field to control $\mathcal{V}^{ab}(\omega)$. Indeed, writing $\mathbf{E}(\omega) = E_0(\omega)(\cos\alpha\hat{\mathbf{x}} + \sin\alpha\hat{\mathbf{y}})$ where α is the polarization angle, we obtain from Eq. (10) that

$$\mathcal{V}^{ab}(\omega, \alpha) = \frac{2}{\hbar\xi(\omega)} \left(\mu^{abxx}(\omega) \cos^2 \alpha + \mu^{abyy}(\omega) \sin^2 \alpha + \mu^{abxy}(\omega) \sin 2\alpha \right) \quad \text{eq:vab-aw} \quad (12)$$

as for the structures chosen in this article, $\xi^{xx}(\omega) = \xi^{yy}(\omega) \equiv \xi(\omega)$, and $\xi^{xy}(\omega) = 0$. Now, we formalize our two options for $\mathcal{V}^{ab}(\omega)$.

A. Fixing spin

sec:theory-fixspin

Analyzing the SVI, Eq. (12), we define the magnitude of the electron velocity in plane with the spin polarized along the b direction as

$$\mathcal{V}_{\sigma^b}(\omega, \alpha) \equiv \sqrt{[\mathcal{V}^{xb}(\omega, \alpha)]^2 + [\mathcal{V}^{yb}(\omega, \alpha)]^2}, \quad \text{eq:vs-mag} \quad (13)$$

and define the angle at which the velocity is directed on the xy plane as

$$\gamma_{\sigma^b}(\omega, \alpha) = \tan^{-1} \left(\frac{\mathcal{V}^{yb}(\omega, \alpha)}{\mathcal{V}^{xb}(\omega, \alpha)} \right). \quad \text{eq:gamma-ang} \quad (14)$$

We also define two special angles

$$\gamma_{\sigma^b}^{\parallel}(\omega, \alpha) = \alpha, \quad \text{eq:gamma-par} \quad (15)$$

and

$$\gamma_{\sigma^b}^{\perp}(\omega, \alpha) = \alpha \pm 90^\circ, \quad \text{eq:gamma-perp} \quad (16)$$

corresponding to the electron velocity being parallel or perpendicular the incoming polarization,

respectively. The subscript σ^b denotes the spin along b.

B. Fixing velocity.

sec:theory-fixvel

Fixing the calculated velocity along $a = x$ or $a = y$ we define it's corresponding magnitude as

$$\mathcal{V}_a(\omega, \alpha) \equiv \sqrt{[\mathcal{V}^{ax}(\omega, \alpha)]^2 + [\mathcal{V}^{ay}(\omega, \alpha)]^2 + [\mathcal{V}^{az}(\omega, \alpha)]^2}, \quad \text{eq:vv-mag} \quad (17)$$

from where we see that the spin would be oriented in the xyz system's coordinates according to a polar angle

$$\theta_a(\omega, \alpha) = \cos^{-1} \left(\frac{\mathcal{V}^{az}(\omega, \alpha)}{\mathcal{V}_a(\omega, \alpha)} \right), \quad 0 \leq \theta \leq \pi, \quad \text{eq:polar-ang} \quad (18)$$

and an azimuthal angle

$$\varphi_a(\omega, \alpha) = \tan^{-1} \left(\frac{\mathcal{V}^{ay}(\omega, \alpha)}{\mathcal{V}^{ax}(\omega, \alpha)} \right), \quad 0 \leq \varphi \leq 2\pi. \quad \text{eq:azimuthal-ang} \quad (19)$$

Layer No.	Atom type	Position (Å)		
		x	y	z
1	H	-0.61516	-1.77416	0.73196
1	H	0.61518	0.35514	0.73175
2	C	-0.61516	-1.77264	-0.49138
2	C	-0.61516	-0.35600	-0.72316
2	C	0.61516	0.35763	-0.49087

TABLE I. Unit cell of Up structure. Layer division, atom types and positions for the Up structure. The structure unit cell was divided in two layers corresponding to hydrogen and carbon atoms. The corresponding layer atom position is depicted in Fig. 1 with the corresponding number of layer tab:up-unitcell

Layer No.	Atom type	Position (Å)		
		x	y	z
1	H	-0.61516	-1.42140	1.47237
2	C	-0.61516	-1.73300	0.39631
3	C	0.61516	1.73300	0.15807
4	C	0.61516	0.42201	-0.15814
5	C	-0.61516	-0.37396	-0.39632
6	H	-0.61516	-0.68566	-1.47237

TABLE II. Unit cell of Alt structure. Layer division, atom types and positions for the Alt structure. The structure unit cell was divided in six layers corresponding each one to atoms in different z positions. The corresponding layer atom position is depicted in Fig. 2 with the corresponding number of layer tab:alt-unitcell

III. RESULTS

`sec:results`

We preset the results of $\mathcal{V}_{\sigma^b}(\omega, \alpha)$ and $\mathcal{V}_a(\omega, \alpha)$ for the $C_{16}H_8$ -up and $C_{16}H_8$ -alt structures being both noncentrosymmetric semi-infinite 2D carbon systems with 50% hydrogenation in different arrangements. We recall that the Up structure has hydrogen atoms only on the upper side of the carbon sheet while the Alt structure has alternating hydrogen atoms on the upper and bottom sides. Also we take the hexagonal carbon lattice to be on the xy plane for both structures, and the carbon-hydrogen bonds on the perpendicular xz plane, as depicted in Figs. 1 and 2. The coordinates for the Up and Alt unit cells of the structures are presented in Tables I and II.

We calculated the self-consistent ground state and the Kohn-Sham states using density functional theory in the local density approximation (DFT-LDA) with a planewave basis using the ABINIT code³⁷. We used Hartwigsen-Goedecker-Hutter (HGH) relativistic separable dual-space Gaussian pseudopotentials³⁸ including the spin-orbit interaction needed to calculate $\mu^{abcd}(\omega, \alpha)$ presented in Eq. (8). The convergence parameters for the calculations of our results corresponding to the Up and Alt structures are cutoff energies of 40 Ha and 65 Ha, resulting in LDA energy band gaps of 0.084 eV and 0.718 eV, respectively. The energy eigenvalues and matrix elements for the Up and Alt structures were calculated using 12802 \mathbf{k} points and 14452 \mathbf{k} points in the IBZ to integrate $\mu^{abcd}(\omega)$ and $\xi^{ab}(\omega)$ using the linearized analytic tetrahedron method (LATM).³⁹ We neglect the anomalous velocity term $\hbar(\boldsymbol{\sigma} \times \nabla V)/4m^2c^2$, where V is the crystal potential, in $\hat{\mathbf{v}}$ of Eq. (1), as this term is known to give small contribution to PSC.¹⁴ Therefore, $[\hat{\mathbf{v}}, \hat{\mathbf{S}}] = 0$ and Eq. (1) reduces to $\hat{K}^{ab} = \hat{v}^a \hat{S}^b = \hat{S}^b \hat{v}^a$. Finally, the prime in the sum of Eq. (8) is restricted to quasidegenerated conduction bands c and c' that are closer than 30 meV, where this value is both a typical laser-pulse energy width and the room-temperature energy.³⁹

A. SVI: Spin velocity injection

`sec:res-spin_velocity`

In Fig. 3, we show $\mathcal{V}^{ab}(\omega, \alpha)$ vs. $\hbar\omega$, for the directions ab and angle α that maximizes the signal, for the Up and Alt structures and for CdSe and GaAs, which are bulk systems shown for comparison. As expected from the delta function of Eq. (8), $\mathcal{V}^{ab}(\omega, \alpha)$ rises right at the corresponding energy gap of each system. For the 2D structures, the spectrum covers two narrow energy regions with large values of the response, while for bulk systems the spectra covers a rather wide energy range, but with a much smaller response. For the Up structure $ab = yz$ and $\alpha = 35^\circ$ maximizes the response, which means that an incoming beam of light with its electric field polarized at 35° from the x direction will induce electrons to move along

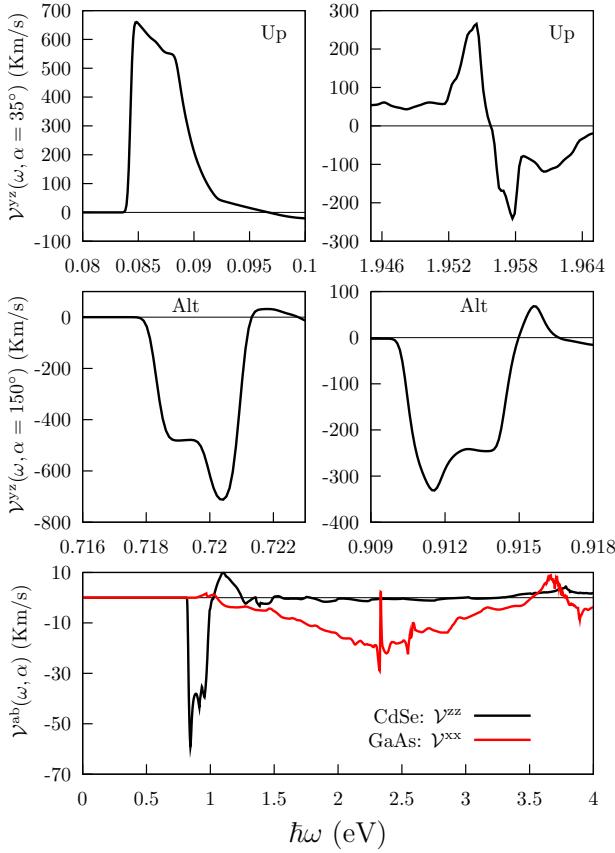


FIG. 3. $\mathcal{V}^{ab}(\omega, \alpha)$ vs. $\hbar\omega$, for the values of α that maximize the signal. The low energy regions for the Alt and Up structures start at the energy gap of each structure, while in the high energy regions, the values of $\mathcal{V}^{ab}(\omega, \alpha)$ are also very large. The bottom panel corresponds to CdSe and GaAs. [fig:vab-str-comp](#)

y (parallel to the surface) with their spin polarized along z (perpendicular to the surface), with the following speeds. Right at the energy onset $\mathcal{V}^{yz}(\omega, \alpha) = 668$ Km/s, speed that remains almost constant for 65 meV, and then goes to zero. A second region is found above 1.946 eV, where there are two extreme values of the speed, $\mathcal{V}^{yz}(\omega, \alpha) = 266.3$ Km/s at $\hbar\omega = 1.954$ eV, and $\mathcal{V}^{ab}(\omega, \alpha) = -241.4$ Km/s at $\hbar\omega = 1.958$ eV; a positive (negative) $\mathcal{V}^{ab}(\omega, \alpha)$ means that the electrons move parallel (antiparallel) to the electric field.

Likewise for the Alt structure we find that also $ab = yz$ and $\alpha = 150^\circ$ maximizes the response, where two extreme values of \mathcal{V}^{yz} are found, one at $\hbar\omega = 0.7204$ eV of $\mathcal{V}^{yz} = -711.9$ Km/s, and the other at $\hbar\omega = 0.911$ eV of $\mathcal{V}^{yz} =$

Structure	Kind of system	Pol. Ang.	Energy [eV]	$\mathcal{V}^{ab}(\omega, \alpha)$ ab [Km/s]
Up	2D	35	0.084	yz 660.5
			1.954	yz 266.3
			1.958	yz -241.4
Alt	2D	150	0.720	yz -711.9
			0.911	yz -330.6
CdSe	bulk	-	0.844	zz -59.0
			2.324	xx -28.7

TABLE III. Comparison of the reported maximum values of $\mathcal{V}^{ab}(\omega, \alpha)$ for the different structures and their corresponding polarization angle α and $\hbar\omega$ energy values.

[tab:vab-str-comp](#)

-330.6 Km/s. For the bulk structures we calculate $\mathcal{V}^{ab}(\omega)$ from Eq. (10) by simply using μ_{\max} . For CdSe we find that for $\hbar\omega = 0.844$ eV, $\mu_{\max} \rightarrow \mu^{zzzz}$, and $\mathcal{V}^{zz}(\omega) = -59.0$ Km/s, and for GaAs at $\hbar\omega = 2.324$ eV, $\mu_{\max} \rightarrow \mu^{aaaa}$ and $\mathcal{V}^{aa}(\omega, \alpha) = -28.7$ Km/s, with $a = x, y, z$. For these bulk semiconductors the x , y , and z axis are taken along the standard cubic unit cell directions, [100], [010], and [001], respectively. In Table III we present the comparison of $\mathcal{V}^{ab}(\omega, \alpha)$ for the 2D structures and bulk crystals. We remark that, as shown in the figure, the 2D structures have maxima in $\mathcal{V}^{ab}(\omega; \alpha)$ that are bigger than for the bulk crystals; in particular the Alt structure gives a $\mathcal{V}^{ab}(\omega; \alpha) \sim 12$ times larger than that of CdSe and GaAs.

B. Fixing spin

[sec:res-fixspin](#)

In this subsection we calculate $\mathcal{V}_{\sigma^z}(\omega, \alpha)$, Eq. (13), for the case where the spin is fixed along z , i.e. directed perpendicularly to the surface of the Up and Alt structures. Also, we calculate $\gamma_{\sigma^z}(\omega, \alpha)$, Eq. (14), that determines the direction along which the injected electrons move along the surface of each structure. We mention that we have also made the analysis for the cases when the spin is directed along x or y , finding similar qualitative results to those presented below.

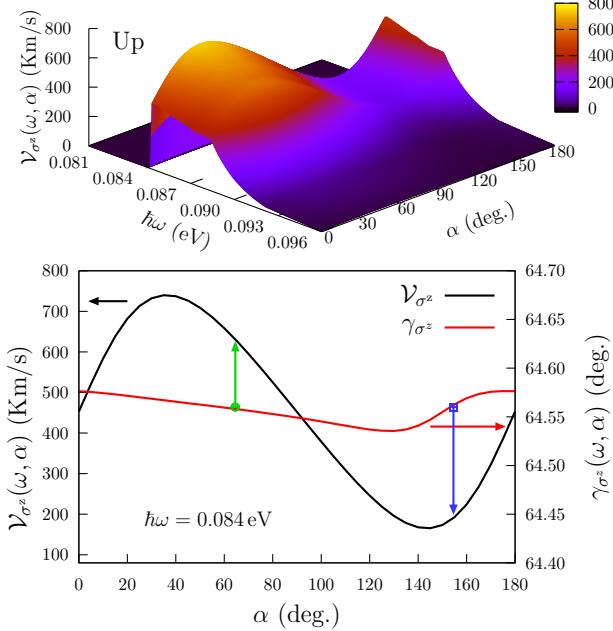


FIG. 4. For the Up structure, the top panel shows $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. $\hbar\omega$ and α , and the bottom panel shows $\gamma_{\sigma^z}(\omega, \alpha)$ (right scale, red line), and $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ (left scale, black line), vs. α , for $\hbar\omega = 0.084$ eV, i.e. along the ridge shown in the 3D plot. fig:up-vs-z-w1

1. Up structure

up:fs

In the top panel of Fig. 4 we plot $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. $0.080 \text{ eV} \leq \hbar\omega \leq 0.096 \text{ eV}$ (same energy range for the Up structure shown in the left panel of Fig. 3) and $0^\circ \leq \alpha \leq 180^\circ$. We see a broad peak that maximizes at $\alpha = 35^\circ$ and $\hbar\omega = 0.084$ eV, with a value of $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 739.7$ Km/s, and that the variation of $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ as a function of α , that comes from the interplay of the μ tensor components as multiplied by the trigonometric functions of Eq. (12), gives a sizable set of values between 739.7 Km/s and 165.4 Km/s, for $0.084 \text{ eV} \leq \hbar\omega \leq 0.090 \text{ eV}$. In the bottom panel, we show $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. α (left scale, black line), at $\hbar\omega = 0.084$ eV, thus following the ridge shown in the 3D plot of the top panel, along with its corresponding velocity angle $\gamma_{\sigma^z}(\omega, \alpha)$ (right scale, red line). It is very interesting to see that $\gamma_{\sigma^z}(\omega, \alpha)$ is centered at 64.55° with a rather small deviation of only $\pm 0.03^\circ$, for the whole range of α . This results means that for $\hbar\omega = 0.084$ eV and for all values of α , the electrons, with the chosen

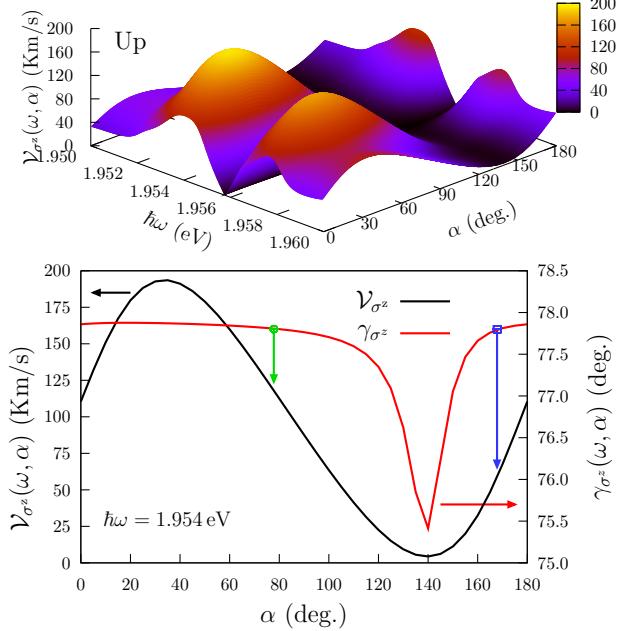


FIG. 5. For the Up structure, the top panel shows $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. $\hbar\omega$ and α , and the bottom panel shows $\gamma_{\sigma^z}(\omega, \alpha)$ (right scale, red line), and $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ (left scale, black line), vs. α , for $\hbar\omega = 1.954$ eV, i.e. along the highest ridge shown in the 3D plot. fig:up-vs-z-w2

spin pointing along z , will move at angle of $\gamma_{\sigma^z}(\omega, \alpha) \sim 64.5^\circ$ with respect to the x direction, with the range of high speeds $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ shown in the figure. Also, from Eq. (15) we find that $\gamma_{\sigma^z}^{\parallel}(\omega, \alpha) = \alpha = 64.56^\circ$, with $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 631.1$ Km/s (see green arrow), and that from Eq. (16), $\gamma_{\sigma^z}^{\perp}(\omega, \alpha) = \alpha - 90^\circ = 64.50^\circ$, gives $\alpha = 154.50^\circ$, with $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 191.5$ Km/s (see blue arrow); thus, at $\hbar\omega = 0.084$ eV, an incident field polarized at $\alpha \sim 65.5^\circ$ or $\sim 154.5^\circ$, injects electrons with their spin polarized along z , that move parallel or perpendicular to the incident electric field, with a speed of 631.14 Km/s or 191.5 Km/s, respectively.

Now, we analyze the results for the second energy range of the Up structure shown in the top right panel of Fig. 3. In the top panel of Fig. 5, we plot $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. $1.950 \text{ eV} \leq \hbar\omega \leq 1.960 \text{ eV}$ and $0^\circ \leq \alpha \leq 180^\circ$. We see two broad peaks that maximize at $\alpha = 35^\circ$ and $\hbar\omega = 1.954$ eV, with a value of $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 193.5$ Km/s, and $\alpha = 35^\circ$ and $\hbar\omega = 1.957$ eV, with a value of $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 170.6$ Km/s. We only analyze the highest maximum in the bottom panel, where we

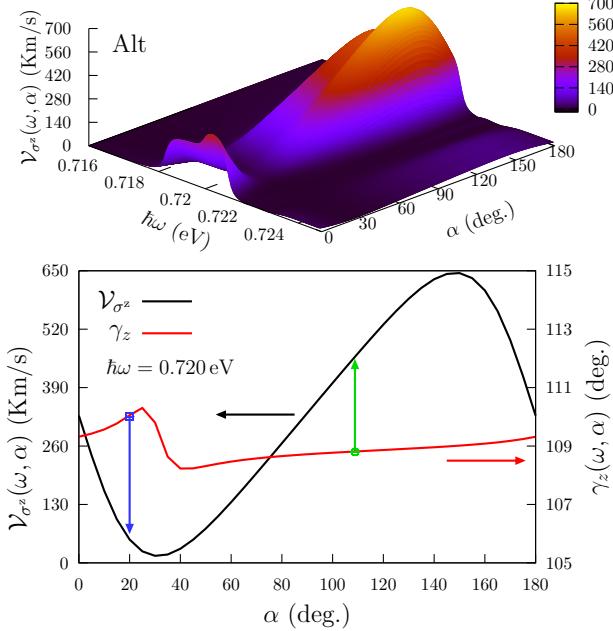


FIG. 6. For the Alt structure, the top panel shows $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. $\hbar\omega$ and α , and the bottom panel shows $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ (right scale, red line), and $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ (left scale, black line), vs. α , for $\hbar\omega = 0.720$ eV, i.e. along the ridge shown in the 3D plot.

fig:alt-vszz

show $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. α (left scale, black line), at $\hbar\omega = 1.954$ eV, thus following the highest ridge shown in the 3D plot of the top panel, **along with its corresponding velocity angle $\gamma_{\sigma^z}(\omega, \alpha)$ (right scale, red line)**. In this case we see that the values of $\gamma_{\sigma^z}(\omega, \alpha)$ have more dispersion, as a function of α , than for the lower energy range shown in the bottom panel of Fig. 4. However, $\gamma_{\sigma^z}(\omega, \alpha) \sim 77.8^\circ$ is constant from $\alpha = 0^\circ$ and up to $\alpha \sim 85^\circ$. In this case, we find that $\gamma_{\sigma^z}^{\parallel}(\omega, \alpha) = \alpha = 78.0^\circ$, with $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 115.0$ Km/s (see green arrow), and that from Eq. (16), $\gamma_{\sigma^z}^{\perp}(\omega, \alpha) = \alpha - 90^\circ = 167.8^\circ$, gives $\alpha = 77.8^\circ$, with $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 65.6$ Km/s (see blue arrow). Thus, by the correct choice of $\hbar\omega$ and α we could inject electrons, in this case with their spin polarized along z , that move parallel or perpendicular to the incident electric field, with finite speeds.

2. Alt structure

We proceed to analyze the Alt structure, just as we did the Up structure, but in this case we

only chose the lower energy range shown in the left central panel of Fig. 3. In the top panel of Fig. 6, we plot $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. 0.715 eV $\leq \hbar\omega \leq 0.725$ eV and $0^\circ \leq \alpha \leq 180^\circ$. We see a broad peak that maximizes at $\alpha = 150^\circ$ and $\hbar\omega = 0.720$ eV, with a value of $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 644.9$ Km/s. In the bottom panel we show $\mathcal{V}_{\sigma^z}(\omega, \alpha)$ vs. α (left scale, black line), at $\hbar\omega = 0.720$ eV, **thus following the highest ridge shown in the 3D plot of the top panel, along with its corresponding velocity angle $\gamma_{\sigma^z}(\omega, \alpha)$ (right scale, red line)**. In this case we see that $\gamma_{\sigma^z}(\omega, \alpha)$ is centered at 109.2° having variations of $\pm 1.0^\circ$ for $0^\circ \leq \alpha \leq 180^\circ$. In this case, we find that $\gamma_{\sigma^z}^{\parallel}(\omega, \alpha) = \alpha = 108.8^\circ$, with $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 450.05$ Km/s (see green arrow), and that from Eq. (16), $\gamma_{\sigma^z}^{\perp}(\omega, \alpha) = \alpha - 90^\circ = 110.0^\circ$, gives $\alpha = 20.0^\circ$, with $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 60.84$ Km/s (see blue arrow). Thus, as for the Up structure, we could inject electrons with a fixed spin that move parallel or perpendicular to the incident electric field.

C. Fixing velocity

sec:res-fixvel

We calculated $\mathcal{V}_a(\omega, \alpha)$ (Eq. (17)) fixing the electron velocity direction, a , to the x or y direction along the surface of the Up and Alt structures. From Eqns. (18) and (19), we determined the polar, $\theta_a(\omega, \alpha)$, and azimuthal, $\varphi_a(\omega, \alpha)$, angles corresponding to the direction of the spin.

1. Up structure

For the Up structure we find once again that $\alpha = 35^\circ$ maximizes the response. In Fig. 7 we plot $\mathcal{V}_a(\omega, \alpha)$ (left scale, black line), $\theta_a(\omega, \alpha)$ (right scale, red line), and $\varphi_a(\omega, \alpha)$, (right scale, blue line), vs. $\hbar\omega$, for $a = x, y$. We see that for $\hbar\omega = 0.084$ eV, the responses has a maximum of $\mathcal{V}_x(\omega, \alpha) = 431.7$ Km/s, with $\theta_x(\omega, \alpha) = 42.5^\circ$, and $\varphi_x(\omega, \alpha) = 208.3^\circ$, and $\mathcal{V}_y(\omega, \alpha) = 687.9$ Km/s, with $\theta_y(\omega, \alpha) = 13.9^\circ$, and $\varphi_y(\omega, \alpha) = 82.1^\circ$. This means that, the spin is directed upward the third Cartesian quadrant of the xy plane when the electron moves along x , and is directed almost parallel to the xy plane in

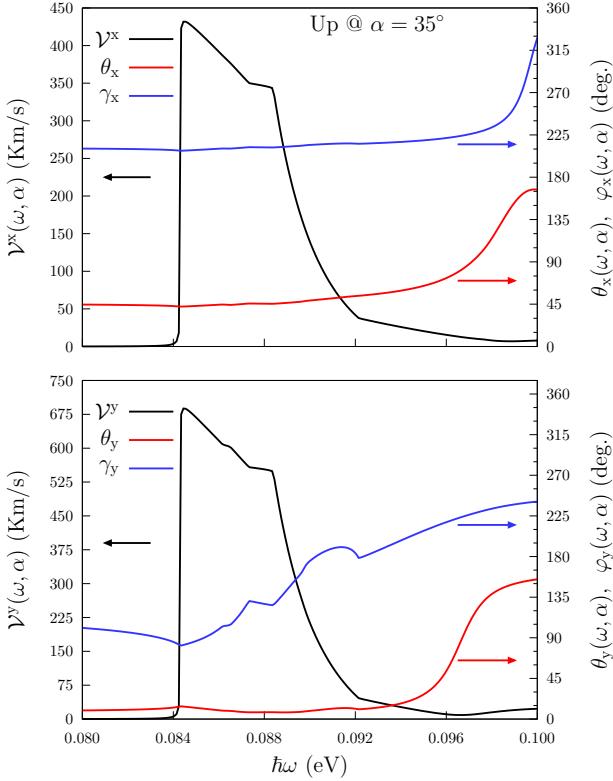


FIG. 7. For the Up structure we show $\mathcal{V}_a(\omega, \alpha)$ (left scale, black line), $\theta_a(\omega, \alpha)$ (right scale, red line), and $\varphi_a(\omega, \alpha)$, (right scale, blue line), vs. $\hbar\omega$, for $\alpha = 35^\circ$, and $a = x, y$.

`fig:up-vab-comp-rtp-1`

the first quadrant when it moves along y . Also, from this figure we have that when the electron moves along x the spin direction is almost constant for all the energies across the peak of the response, having $42.5^\circ < \theta_x(\omega, \alpha) < 53.7^\circ$ and $208.3^\circ < \varphi_x(\omega, \alpha) < 215.7^\circ$, and when the electron moves along y the spin polar angle has again small variations, $11.3^\circ < \theta_y(\omega, \alpha) < 13.9^\circ$, but the azimuthal angle has significant variations, $82.1^\circ < \varphi_y(\omega, \alpha) < 182.4^\circ$.

In Fig. 8 we plot $\mathcal{V}_a(\omega, \alpha)$ vs. $\hbar\omega$, in the range where there are two local maxima at $\hbar\omega = 1.954$ eV and $\hbar\omega = 1.957$ eV. The former is the largest of the two, with $\mathcal{V}_x(\omega, \alpha) = 61.2$ Km/s, $\theta_x(\omega, \alpha) = 48.3^\circ$, and $\varphi_x(\omega, \alpha) = 54.3^\circ$, for the electron moving along x , and $\mathcal{V}_y(\omega, \alpha) = 263.7$ Km/s, $\theta_y(\omega, \alpha) = 49.8^\circ$, and $\varphi_y(\omega, \alpha) = 230.7^\circ$ for the electron moving along y . For the $\hbar\omega = 1.957$ eV peak we obtain $\theta_x(\omega, \alpha) = 129.8^\circ$, and $\varphi_x(\omega, \alpha) = 231.7^\circ$, with $\mathcal{V}^x(\omega, \alpha) = 54.6$ Km/s, and $\theta_y(\omega, \alpha) =$

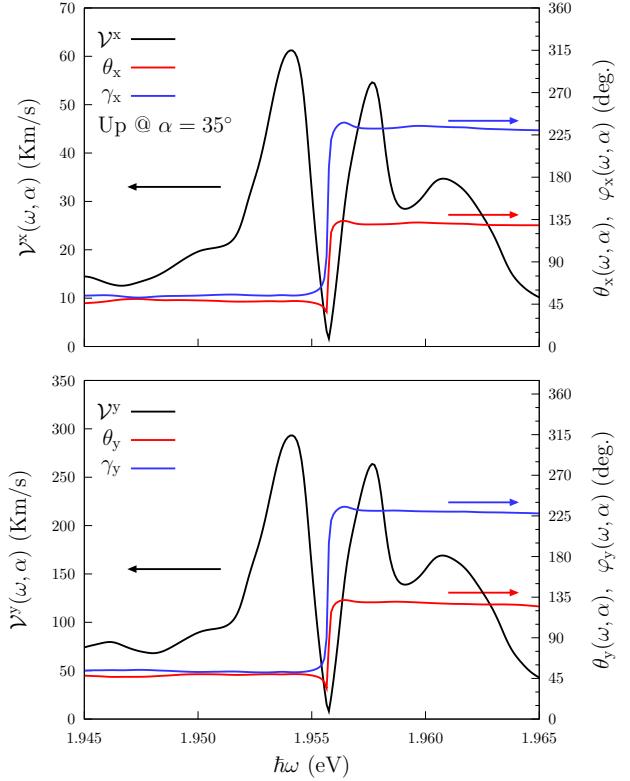


FIG. 8. For the Up structure we show $\mathcal{V}_a(\omega, \alpha)$ (left scale, black line), $\theta_a(\omega, \alpha)$ (right scale, red line), and $\varphi_a(\omega, \alpha)$, (right scale, blue line), vs. $\hbar\omega$, for $\alpha = 35^\circ$, and $a = x, y$.

`fig:up-vx-vy-w2`

129.3, and $\varphi_y(\omega, \alpha) = 230.7$, with $\mathcal{V}^y(\omega, \alpha) = 263.7$ Km/s. **Checar que esto sea correcto para ambos maximos!!** We remark that these angles are almost constant for all the energy values across the peak of this two local maxima, for which the spin is directed upward in the first Cartesian quadrant of the xy plane when it moves along either x or y directions.

2. Alt structure

In Figs. 9 and 10 we plot $\mathcal{V}_a(\omega, \alpha)$ (left scale, black line), $\theta_a(\omega, \alpha)$ (right scale, red line), and $\varphi_a(\omega, \alpha)$, (right scale, blue line), vs. $\hbar\omega$ in two different ranges, and for $a = x, y$. In this case, $\alpha = 150^\circ$, maximizes both $\mathcal{V}_x(\omega, \alpha)$, and $\mathcal{V}_y(\omega, \alpha)$, as a function of α . In Fig. 9 the absolute maxima is at $\hbar\omega = 0.7204$ eV, with $\mathcal{V}_x(\omega, \alpha) = 301.7$ Km/s, $\theta_x(\omega, \alpha) = 44.5^\circ$, and $\varphi_x(\omega, \alpha) = 51.2^\circ$, and $\mathcal{V}_y(\omega, \alpha) = 905.6$ Km/s, with $\theta_y(\omega, \alpha) = 119.7^\circ$, and $\varphi_y(\omega, \alpha) = 163.4^\circ$.

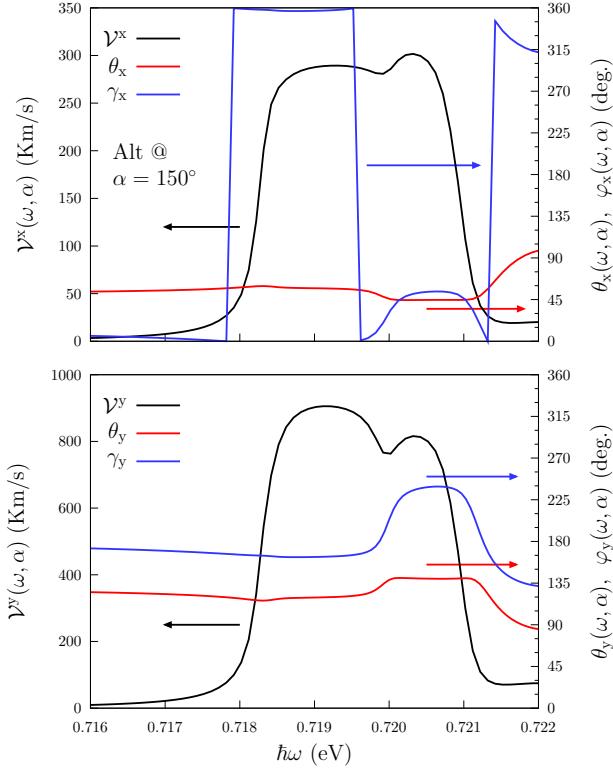


FIG. 9. For the Alt structure we show $\mathcal{V}_a(\omega, \alpha)$ (left scale, black line), $\theta_a(\omega, \alpha)$ (right scale, red line), and $\varphi_a(\omega, \alpha)$, (right scale, blue line), vs. $\hbar\omega$, for $\alpha = 150^\circ$, and $a = x, y$.

`fig:alt-vx-vy-w1`

Thus, the spin is directed upward the forth Cartesian quadrant of the xy plane when the spin velocity is directed along x , and directed downward the second Cartesian quadrant when the spin velocity is directed along y . Finally, in Fig. 9, the absolute maxima is at $\hbar\omega = 0.911$ eV, with $\mathcal{V}_x(\omega, \alpha) = 276.3$ Km/s, $\theta_x(\omega, \alpha) = 154.6^\circ$, and $\varphi_x(\omega, \alpha) = 292.3^\circ$, and $\mathcal{V}_y(\omega, \alpha) = 468.6$ Km/s, with $\theta_y(\omega, \alpha) = 129.2^\circ$, and $\varphi_y(\omega, \alpha) = 228.3^\circ$, implying that the spin is directed downward the forth Cartesian quadrant of the xy plane when the spin velocity is directed along x , and directed downward the third Cartesian quadrant when the spin velocity is directed along y .

IV. CONCLUSIONS

`sec:conclusions`

We have performed an *ab initio* calculation for the SVI by one-photon absorption of linearly polarized light in the Up and Alt 2D hydro-

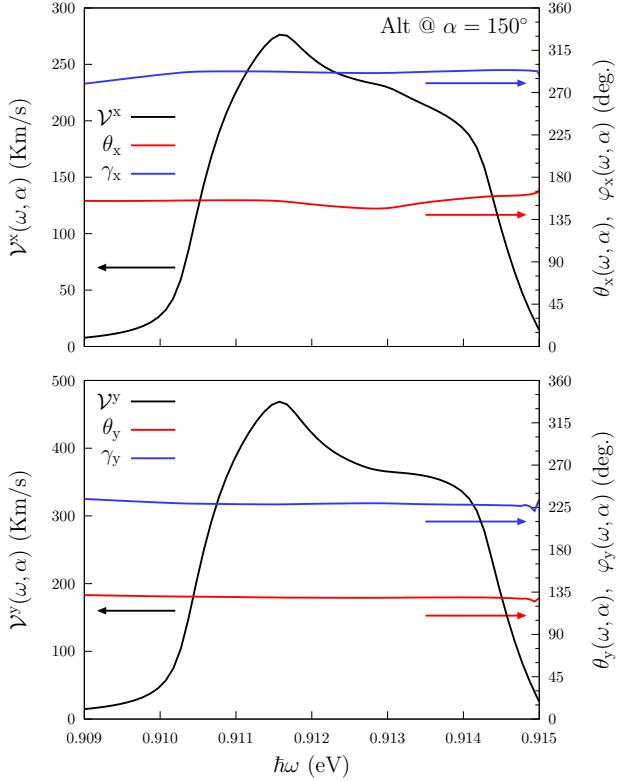


FIG. 10. For the Alt structure we show $\mathcal{V}_a(\omega, \alpha)$ (left scale, black line), $\theta_a(\omega, \alpha)$ (right scale, red line), and $\varphi_a(\omega, \alpha)$, (right scale, blue line), vs. $\hbar\omega$, for $\alpha = 150^\circ$, and $a = x, y$.

`fig:alt-vx-vy-w2`

generated graphene structures that and we made the calculation for the case when the spin is polarized in the z direction or when the velocity is directed along x or y ; this effect does not seem to have been reported previously. This SVI is very sensitive to the symmetry characteristics of the structures presenting an anisotropic behavior. We found that the Up structure has the most intense response for the spin directed along z resulting in $\mathcal{V}_{\sigma^z}(\omega, \alpha) = 668.0$ Km/s and for an energy of the incoming beam of 0.084 eV. Also the Alt structure has the most intense response when the spin moves along the y direction resulting in $\mathcal{V}^y(\omega, \alpha) = 905.6$ Km/s for an energy of the incoming beam of 0.720 eV. The spin relaxation time in pure and doped graphene is long enough in the order from nanoseconds to milliseconds.^{40,41} The, according to our results both are excellent candidates for the development of spintronics devices that require PSC due to the high spin velocity transport.

V. ACKNOWLEDGMENT

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