FirstPage

Pure Spin Current Injection in Hydrogenated Graphene Structures

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(Dated: May 11, 2017)

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I. INTRODUCTION

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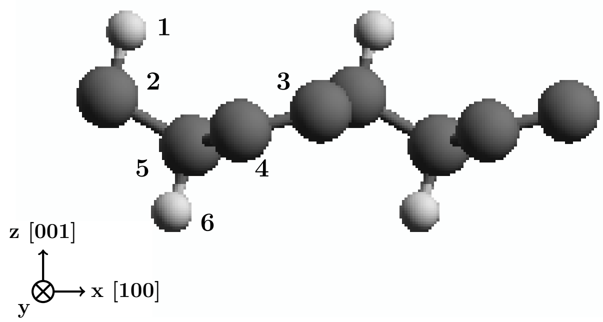
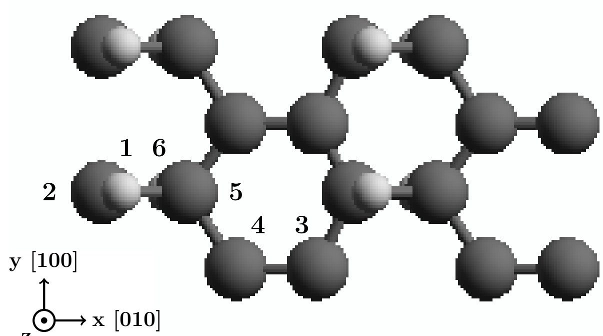


(a) xz plane view fig:alt-struc-xz



(b) xy plane view fig:alt-struc-xy

FIG. 1. Alt structure. fig:alt-struc

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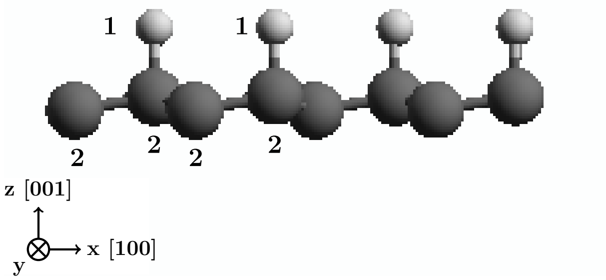
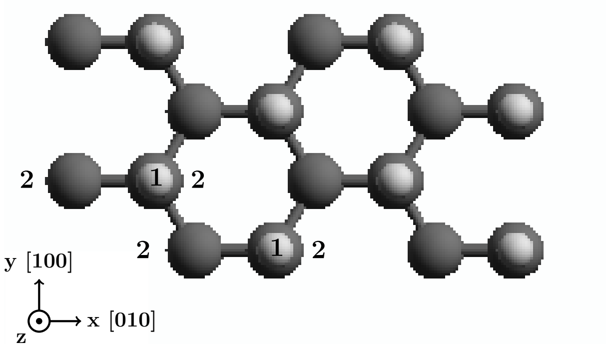


(a) xz plane view fig:up-struc-xz



(b) xy plane view fig:up-struc-xy

FIG. 2. Up structure fig:up-struc

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II. THEORY

sec:theory

A. Pure spin velocity

sec:theory-pure_spin_current

The spin density injection current $\dot{K}^{\mathrm{ab}}$ with speed along direction a and spin polarization along b is defined as

$$\dot{K} = \mu^{\mathrm{abcd}}(\omega) E^{\mathrm{c}}(\omega) E^{\mathrm{d}*}(\omega) \tag{1}$$

eq:dotk

de las notas q te di tienes que
hacer esta seccion clara, corta, y
con las explicacion fisica de lo que
se esta haciendo.

$$(\omega) = \ldots \frac{\ldots}{\hbar^2} \int \frac{\ldots}{8\pi^3} \sum_{vcc'} \Big[\ldots (\ldots r_{cv} + r^{\mathrm{d}}_{vc'} r^{\mathrm{c}}_{cv}) \Big] \delta(\omega - \omega_{cv}) \tag{2}$$

eq:mu

$$K^{\mathrm{ab}}_{mn} = \sum_{\ell} v^{\mathrm{a}}_{nl} S^{\mathrm{b}}_{lm} \tag{3}$$

eq:velspi-matelem

is the corresponding spin density injection current pseudotensor. The $'$ in the sum means that

c and c' are quasi degenerate states and the sum only covers these states.

Now we define the spin velocity, $\mathcal{V}^{\mathrm{ab}}$ as the speed at which the spin polarized in the b direction moves along the a direction when a normal incident beam reaches the xy plane with a polarization angle α. Then,

$$\mathcal{V}^{\mathrm{ab}}(\omega) = \frac{2}{\hbar}\frac{\mu^{\mathrm{abxx}}(\omega)E^2(\omega)\cos^2(\alpha) + \mu^{\mathrm{abyy}}(\omega)E^2(\omega)\sin^2(\alpha) + 2\mu^{\mathrm{abxy}}(\omega)E^2(\omega)\cos(\alpha)\sin(\alpha)}{\xi^{\mathrm{xx}}(\omega)E^2(\omega)\cos^2(\alpha) + \xi^{\mathrm{yy}}(\omega)E^2(\omega)\sin^2(\alpha)},$$
$$= \frac{2}{\hbar}\frac{\mu^{\mathrm{abxx}}(\omega)\cos^2(\alpha) + \mu^{\mathrm{abyy}}(\omega)\sin^2(\alpha) + \mu^{\mathrm{abxy}}(\omega)\sin(2\alpha)}{\xi^{\mathrm{xx}}(\omega)\cos^2(\alpha) + \xi^{\mathrm{yy}}(\omega)\sin^2(\alpha)}. \quad \texttt{eq:vab} \quad (4)$$

For an angle $\alpha = \frac{\pi}{4}$ this expression can be reduced to

$$\mathcal{V}^{\mathrm{ab}}(\omega) = \frac{2}{\hbar}\frac{\mu^{\mathrm{abxx}}(\omega) + \mu^{\mathrm{abyy}}(\omega) + 2\mu^{\mathrm{abxy}}(\omega)}{\xi^{\mathrm{xx}}(\omega) + \xi^{\mathrm{yy}}(\omega)}. \quad \texttt{eq:vab-90deg} \quad (5)$$

B. Fixing spin

falta dar el sentido fisico
de estas cantidades.

`fixspin`

C... we can fi... and z Carte... the magnitude of the spin velocity $|\mathcal{V}_{\sigma^{\mathrm{b}}}|$ in a fixed angle γ_b as

$$|\mathcal{V}_{\sigma^{\mathrm{b}}}|(\omega) = \sqrt{(\mathcal{V}^{\mathrm{ax}}(\omega))^2 + (\mathcal{V}^{\mathrm{ay}}(\omega))^2}, \quad \texttt{eq:vs-mag} \quad (6)$$
$$\gamma_{\mathrm{b}}(\omega) = \tan^{-1}\left(\frac{\mathcal{V}^{\mathrm{ay}}(\omega)}{\mathcal{V}^{\mathrm{ax}}(\omega)}\right), \quad \texttt{eq:gamma-ang} \quad (7)$$

where the angle is measured in the counter-clockwise direction from the positive x axis.

C. Fixing velocity.

`sec:theory-fixvel`

In a similar way we can fix the velocity in the xy plane along x and y directions and define $|\mathcal{V}^{\mathrm{a}}|$ as

$$|\mathcal{V}^{\mathrm{a}}|(\omega) = \sqrt{(\mathcal{V}^{\mathrm{ax}}(\omega))^2 + (\mathcal{V}^{\mathrm{ay}}(\omega))^2 + (\mathcal{V}^{\mathrm{az}}(\omega))^2}, \quad \texttt{eq:vv-mag} \quad (8)$$

and the corresponding polar and azimuthal angles θ and φ as

$$\theta_{\mathrm{a}}(\omega) = \cos^{-1}\left(\frac{\mathcal{V}^{\mathrm{az}}(\omega)}{|\mathcal{V}^{\mathrm{a}}(\omega)|}\right), \quad 0 \leq \theta \leq \pi, \quad \texttt{eq:polar-ang} \quad (9)$$
$$\varphi_{\mathrm{a}}(\omega) = \tan^{-1}\left(\frac{\mathcal{V}^{\mathrm{ay}}(\omega)}{\mathcal{V}^{\mathrm{ax}}(\omega)}\right), \quad 0 \leq \varphi \leq 2\pi. \quad \texttt{eq:azimuthal-ang} \quad (10)$$

D. Layer-by-layer analysis.

`sec:theory-layer`

For a layered system we have that the total contribution of Eqns. (6) and (8) is given[1] by

$$|\mathcal{V}_{\sigma^{\mathrm{b}}}(\omega)| = \ell_{\mathrm{eff}}\sum_{\ell=1}^{N_{\mathrm{eff}}}|\mathcal{V}_{\sigma^{\mathrm{b}}}(\ell|\omega)| \quad \texttt{eq:vs-layer} \quad (11)$$
$$|\mathcal{V}^{\mathrm{a}}(\omega)| = \ell_{\mathrm{eff}}\sum_{\ell=1}^{N_{\mathrm{eff}}}|\mathcal{V}^{\mathrm{a}}(\ell|\omega)| \quad \texttt{eq:vv-layer} \quad (12)$$

III. RESULTS

dendtro
de | |

`...ts`

2D

We preset the results for $|\mathcal{V}^{\mathrm{a}}|(\omega)$ and $|\mathcal{V}_{\sigma^{\mathrm{b}}}|($... for the $C_{16}H_8$-alt and $C_{16}H_8$-up structures... ing both noncentrosymmetric semi-infinite carbon systems with 50% hydrogenation in different arrangements. The *alt* system has alternating hydrogen atoms on the upper and bottom sides of the carbon sheet, while the *up* system has H only on the upper side. 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.

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 I. 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. 1 with the corresponding number of layer. `tab:alt-unitcell`

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 II. 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 correspondi... ...on is depicted in Fig. 2 with ... ...r of layer. `tab:up-unitcell`

comienza con
el metodo de
calculo

Us... ...ode[2] 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. We used Hartwigsen-Goedecker-Hutter (HGH) relativistic separable dual-space Gaussian pseudopotentials[3] including the spin-orbit interaction needed to calculate $\mu^{\rm abcd}(\omega)$ (Eq. (2)), ~~$\mathcal{V}^{\rm ab}(\omega)$ (Eq. (4)), $|\mathcal{V}_{\sigma^{\rm b}}|(\omega)$ (Eq. (6)) and |... (8)).~~ It is known that using D... ...the electronic structure of... ...different band gap than the e... ...tally. A correction for the band gap energy value can be calculated by other *ab-initio* methods such as the GW approximation[4] but this is outside the scope of this paper. The convergence parameters for the

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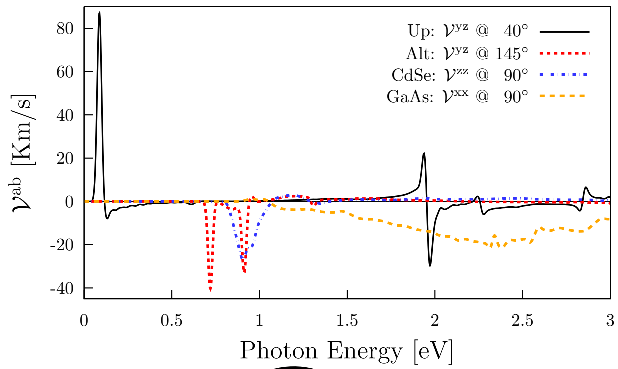


bulk

FIG. 3. Comparison ... ...ntense responses of $\mathcal{V}^{\rm ab}$ for *alt*, *up*, CdSe, and GaAs structures and the corresponding polarization angles. `fig:vab-str-comp`

calculations of our results corresponding to the *alt* and *up* structures are cutoff energies of 65 Ha and 40 Ha, respectively. The energy eigenvalues and matrix elements were calculated using 14452 **k** points and 8452 **k** points in the irreducible Brillouin zone (IBZ) and present LDA energy band gaps of 0.72 eV and 0.088 eV, respectively for the *alt* and *up* structures.

pon cual es,
la expression!

`...res-spin_velocity`

como se escoge
alpha?

In figure 3 we p... ...ison of the most intense re... ...luate the Eq. (4) for t... ...es vs. CdSe and GaAs bulk sys... ...As we can see from this figure the most intense response corresponds to the *up* structure centered at 0.088 eV corresponding to the THz radiation and reaching a spin velocity of 87.2 Km/s. In the other hand,

Structure	Kind of system	Pol. Ang.	Energy [eV]	$\mathcal{V}^{\rm ab}(\omega)$ ab	[Km/s]
up	2D	40	0.09	yz	87.16
			1.94	yz	22.22
			1.97	yz	-29.70
alt	2D	145	0.72	yz	-40.21
			0.91	yz	-32.89
CdSe	bulk	90	0.91	zz	-26.87
GaAs	bulk	90	2.31	xx	-21.62

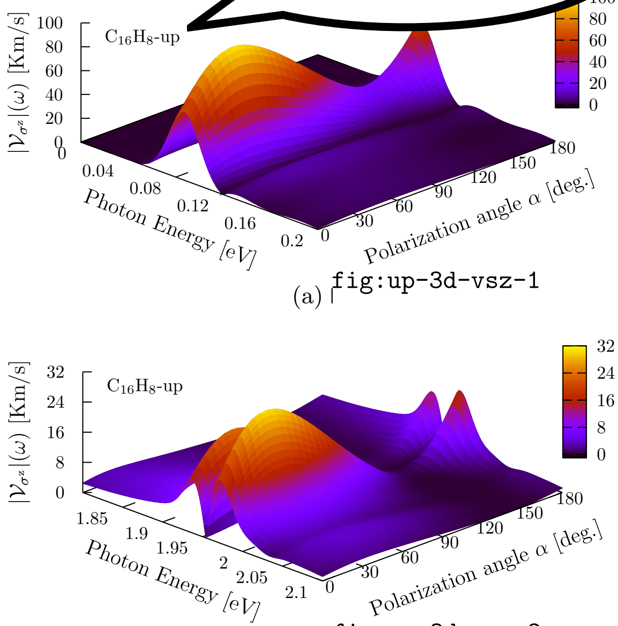
TABLE III. Comparison of the reported maxima values of $\mathcal{V}^{\rm ab}$ for different structures and the corresponding polarization angle α and energy values. `tab:Vab-str-comp` for an energy range from 0.66 eV to ? eV, corresponding to energies of the Thz and visible radiation, all the four structures have contributions in the same order of magnitude. Starting with the 2D structures we have that the *up* structure has other two peaks centered at 1.94 eV and 1.97 eV reaching spin velocities of 22.2 Km/s and -2 que significa el menos? ively, and the *alt* structure tered at 0.72 eV and 0.91 e velocities of -40.2 Km/s and -32.9 Km/s, respectively. Then, for the bulk structures we have that the CdSe has only one intense response centered at 0.91 eV reaching a spin velocity of -26.9 Km/s, and the GaAs structure has a large and almost planar zone where the response is held reaching the maximum for an incoming beam of ene V and resulting in a spin velocit concluir algo sesudo ble III we present the comp s for the 2D and bulk structures.

B. Fix expresion!! spin

Up structure

We first analyzed two energy ranges for the *up* structure, the first for an incoming energy beam from 0.0 eV to 0.2 eV in the THz radiation range, where the absolute maximum of the $|\mathcal{V}_{\sigma^z}|(\omega)$ response is obtained and the second for an energy range from 1.80 eV to 2.1 eV, corresponding to the THz and visible radiation, where two local maxima ar ig. 4 we present the $|\mathcal{V}_{\sigma^z}|(\omega)$ va en la descripcion de la Fig. 3 m evaluate Eq. (6) using d gles α in Eq. (4). From at the onset of the respon e energy of the incoming beam is the same of the gap energy. Making the analysis, we obtained that the zone where the maximum response is held corresponds to a energy range of the incident beam from 0.084 eV to 0.093 eV and polarization angles α between 30° and 45°. Also two local maxima are held for same polarization angles but for an energy range of the incoming beam between 1.90 eV and 2.05 eV. In the top frames of Figs.5(a) and 5(b) we present in solid lines the result of evaluate $|\mathcal{V}_{\sigma^z}|(\omega)$, related to the left scale, fixing the energy of the incoming

falta una descripcion mas detallada

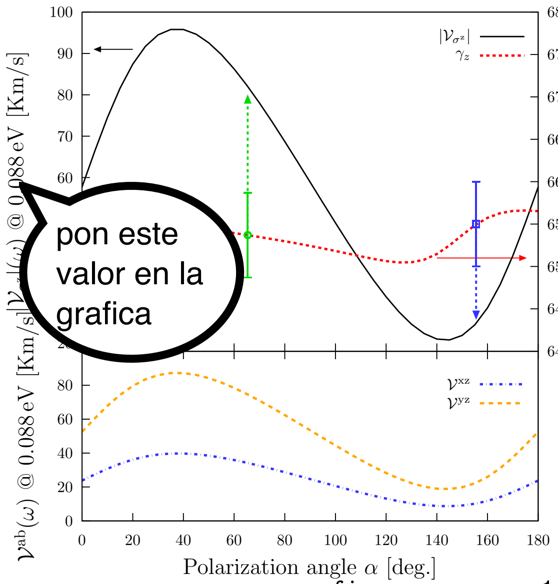


(a) fig:up-3d-vsz-1

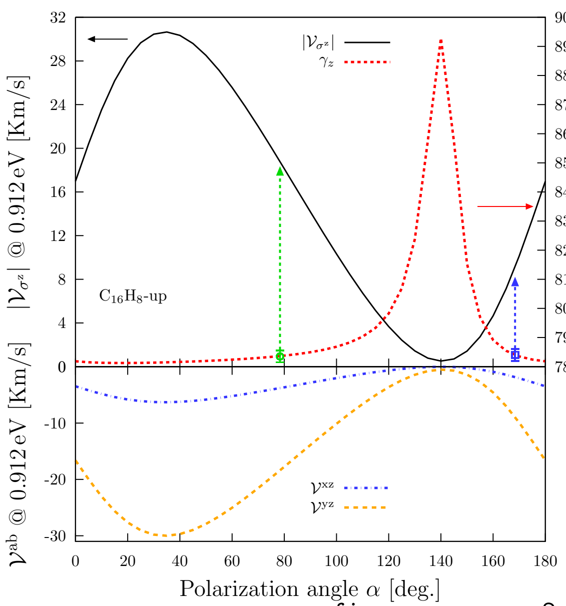
(b) fig:up-3d-vsz-2

FIG. 4. $|\mathcal{V}_{\sigma^z}|(\omega)$, response vs. photon energy vs. polarization angle α for the *up* structure for two energy ranges. The absolute maxima is located for an energy range from 0.08 eV to 0.10 eV and the local maximum from 1.95 eV to 2.0 eV and both for polarization angles between 25° and 50°. fig:up-3d-vsz

beam to 0.088 eV and 0.912 eV, respectively, for which value the response is maximized for the *up* structure. In the same figures and frames we present in dashed lines, related to the right scale, the corresponding velocity angle $\gamma_z(\omega)$ obtained from t Eq. (7), and in the bott explicar con detalle y cerciorate que sea correcto he correspondi). Also we prese xes indicating th les of the spin velocity are parallel and perpendicular and the arrows are directed to the value of the response corresponding to those angles. From Figs. 4(a) and 5(a) we have that the absolute maximum response for the *up* structure is obtained for an incoming beam with energy of 0.088 eV and polarization angle $\alpha = 40°$ resulting in a value of $|\mathcal{V}_{\sigma^z}|(\omega) = 95.8$ Km/s coming from the contribution of the components $\mathcal{V}^{xz}(\omega) = 39.8$ Km/s and $\mathcal{V}^{yz}(\omega) = 87.2$ Km/s for the spin polarized in the z direction and having a velocity angle $\gamma_z(\omega) = 65°$ on the xy plane. In the same fig-



(a) fig:up-vaz-rag-1



(b) fig:up-vaz-rag-2

FIG. 5. Most intense response of $|\mathcal{V}_{\sigma^z}|(\omega)$ (top frames, right scale of figs (a) and (b)), the corresponding velocity angle $\gamma_z(\omega)$ (top frames, right scale), the collinear (circled box) and perpendicular (square box) angles, and the two components $\mathcal{V}^{xz}(\omega)$ and $\mathcal{V}^{yz}(\omega)$ (bottom frames) for the *up* structure fixing the energy to 0.088 eV. fig:up-vaz-rag

ure the green circled box indicates the value for which the polarization angle α and the response direction angle $\gamma_z(\omega)$ are collinear being both angle 65.5° and resulting in a value of the response of $|\mathcal{V}_{\sigma^z}|(\omega) = 82.3$ Km/s indicated by the upward green arrow. Also the blue square box indicates the value for which the polarization angle and the response angle are perpendicular being $\alpha = 155.5°$ and $\gamma_x(\omega) = 65.5°$; for this angles the response has a value of $|\mathcal{V}_{\sigma^z}|(\omega) = 24.8$ Km/s indicated by the blue downward arrow. The green and blue error bars are fixed for a value of $\pm 0.5°$ and then, for variations of this magnitude in $\gamma_z(\omega)$ the complete range of α angle is included because this last is almost constant. Now from Figs. 4(b) and 5(b) we have that a local maxima of the response is obtained for an incoming beam with energy of 0.912 eV and same polarization angle $\alpha = 40°$ resulting in a value of $|\mathcal{V}_{\sigma^z}|(\omega) = 30.3$ Km/s. This comes from a major contribution of the $\mathcal{V}^{yz}(\omega)$ component being directed in a velocity angle $\gamma_z(\omega) = 78°$ on the first Cartesian Quadrant of the xy plane, for the spin polarized in the z direction. Again the green circled box indicate[…] polarization angle α […] angle $\gamma_z(\omega)$ are colline[…] having a response value of $|\mathcal{V}_{\sigma^z}|(\omega) = 23.5$ Km/s indicated with the green upward arrow. We found that for variations in the response angle of $\pm 2°$, indicated with the error bars, corresponds a range in the polarization angle of $0° \leq \alpha \leq 122°$ having then a large range for which the direction of the response is directed to this angle. The blue square box indicates the value for which the polarization angle and the response angle are perpendicular being $\alpha = 168.5°$ $\gamma_z(\omega) = 78.5°$ and having a response $|\mathcal{V}_{\sigma^z}|(\omega) = 9.0$ Km/s indicated with the blue upward arrow. Again, for variations in the response angle of $\pm 2°$, indicated with the error bars, corresponds a range in the polarization angle of $155° \leq \alpha \leq 180°$ […] again a large range for which t[…]se is held. The most […]pin is perpendicular […]ure and also for the […] intense was the presented before for which the spin is polarized in the z direction. We also made the analysis for the cases when the spin polarization is directed in the x and y direction but we do not present the corresponding plots. For those cases we have that the absolute maxima response is obtained for an energy of the incoming beam equal to 0.088 eV and polarization angle $\alpha = 40°$

no se entiende/
no esta claro

mencionar donde
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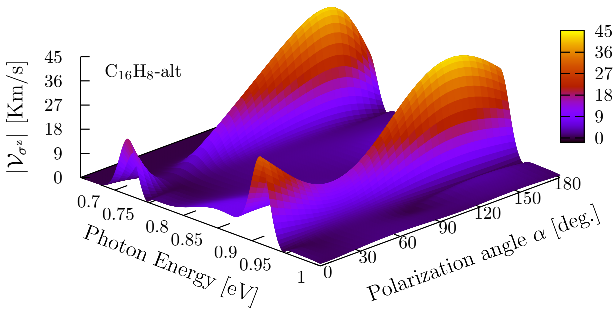


FIG. 6. $|\mathcal{V}_{\sigma^z}|(\omega)$, response vs. photon energy vs. polarization angle α for the *alt* structure. The absolute maximum is located for an energy range from 0.90 eV to 0.93 eV and for polarization angles between 120° and 150°. `fig:alt-3d-vsb`

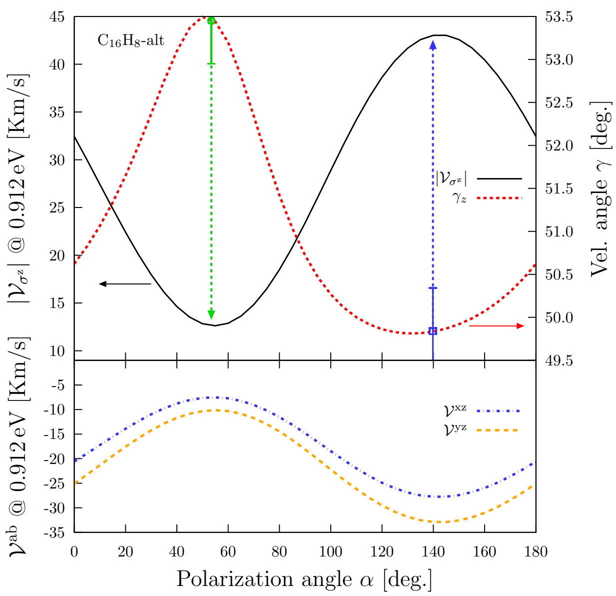


FIG. 7. Most intense response of $|\mathcal{V}_{\sigma^z}|(\omega)$ (top frame, left scale) the corresponding velocity angle $\gamma_z(\omega)$ (top frame, right scale), the collinear (circled box) and perpendicular (square box) angles, and the two components $\mathcal{V}^{xz}(\omega)$ and $\mathcal{V}^{yz}(\omega)$ (bottom frame) for the *alt* structure fixing the energy to 0.912 eV. `fig:alt-vaz-rag`

resulting in values of $|\mathcal{V}_{\sigma^x}|(\omega) = 37.4$ Km/s and $|\mathcal{V}_{\sigma^y}|(\omega) = 24.8$ Km/s.

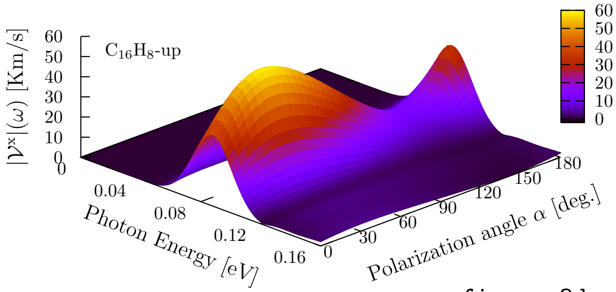
Alt structure

For the *alt* structure ? analyzed the energy range for the incid m from 0.6 eV to 1.0 eV, corresponding to the THz radiation, where the absolute maximum of $|\mathcal{V}_{\sigma^z}|(\omega)$ response is obtained. In Fig. 6 we present the $|\mathcal{V}_{\sigma^z}|(\omega)$ spectra resulting from evaluate again Eq. (6) using different polarization angle α in

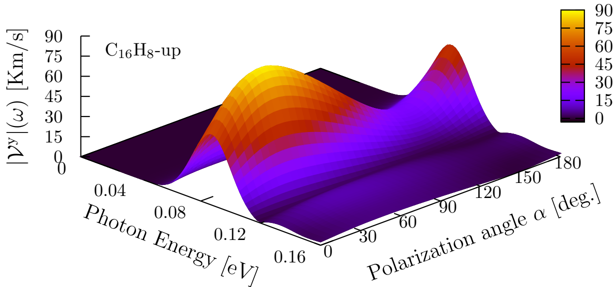
as a function of

Eq. (4) for the *alt* structure. ~~In the figure we have that the onset of the response starts when the energy of the incoming beam is the same of the gap energy.~~ From this figure we found that the zone where the absolute maximum response is held corresponds to a energy range from 0.90 eV to 0.93 eV and polarization angles α between 120° and 150°. Also, a local maximum is obtained for the same polarization angles but for energies between 0.67 eV and 0.75 eV. In the top frame of Fig. 7 we present in solid line the result of evaluate $|\mathcal{V}_{\sigma^z}|(\omega)$, related to the left scale, fixing the energy of the incoming beam to 0.912 eV for which value the response is maximized for the *alt* structure. In the same figure and frame we present with dashed line, related to the right scale, the velocity angle $\gamma_z(\omega)$ and in the bottom frame the corresponding $\mathcal{V}^{xz}(\omega)$ and $\mathcal{V}^{yz}(\omega)$ components. Again, the circled and square boxes indicate the values for which the polarization ... velocity angle are parallel ... arrows are ind... e value. Fro... have that th... r the *alt* struct... ing beam with polarization ang... 145° reaching a velocity of $|\mathcal{V}_{\sigma^z}|(\omega) = 43.0$ Km/s and for the spin polarized in the z direction and resulting in a velocity angle $\gamma_z(\omega) = 50°$ on the first Cartesian Quadrant of the xy plane. The circled box for the collinear angle corresponds for angles α and $\gamma_z(\omega)$ equal to 53.5° with a value of $|\mathcal{V}_{\sigma^z}|(\omega) = 12.7$ Km/s, and the blue square box indicates the perpendicular angles for values $\alpha = 140°$ and $\gamma_z(\omega) = 50°$ with a value of $|\mathcal{V}_{\sigma^z}|(\omega) = 43$ Km/s. Finally we found that for variations of $\pm 0.5°$ of those collinear and perpendicular angles, presented with the error bars on the boxes, correspond ranges for the polarization angle $30° \leq \alpha \leq 70°$ and $95° \leq \alpha \leq 175°$ covering a wide range of angles because the response angle $\gamma_z(\omega)$ has small variations for the complete range of the polarization angle α. Again, for the cases in which the spin polarization is parallel to the surface of the *alt* structure was calculated but the plots are not presented here. The absolute maxima for the case when the spin polarization is directed in the x and y direction are ob-

la explicacion es como la de up, asi que tal vez solo damos los resultados

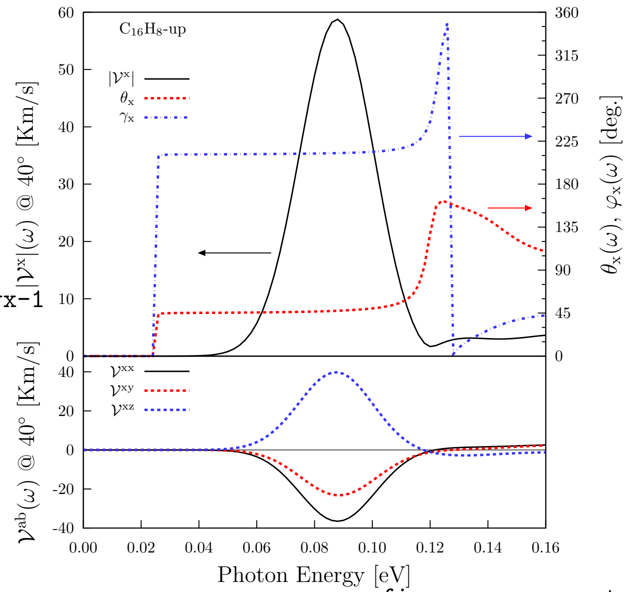


(a) $|\mathcal{V}^{x}|(\omega)$ for *up* structure fig:up-3d-vvx-1

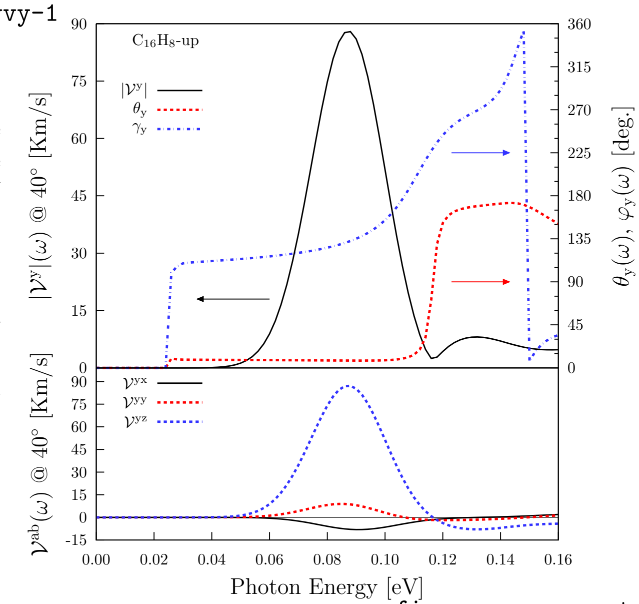


(b) $|\mathcal{V}^{y}|(\omega)$ for *up* structure fig:up-3d-vvy-1

FIG. 8. $|\mathcal{V}^{a}|(\omega)$ response vs. photon energy vs. polarization angle for the *up* structure. The absolute maxima of both responses $|\mathcal{V}^{x}|(\omega)$ and $|\mathcal{V}^{y}|(\omega)$ are localized in the energy range from 0.08 eV to 0.10 eV and for polarization angles from 25° to 50°. fig:up-3d-vva-1



(a) $|\mathcal{V}^{x}|(\omega)$ fig:up-vx-comp-rtp-1



(b) $|\mathcal{V}^{y}|(\omega)$ fig:up-vy-comp-rtp-1

FIG. 9. Most intense response of $|\mathcal{V}^{x}|(\omega)$ and $|\mathcal{V}^{y}|(\omega)$ (top frames left scale of Figs. (a) and (b)), the corresponding polar φ and azimuthal θ angles (top frames right scale), and the corresponding three components (bottom frames) for the *up* structure fixing the polarization angle to $\alpha = 40°$ to maximize the response. fig:up-vab-comp-rtp-1

tained for an energy of the incoming beam equal to 0.912 eV and polarization angle $\alpha = 145°$ resulting in values of $|\mathcal{V}_{\sigma^x}|(\omega) = 27.1$ Km/s and $|\mathcal{V}_{\sigma^y}|(\omega) = 33.2$ Km/s.

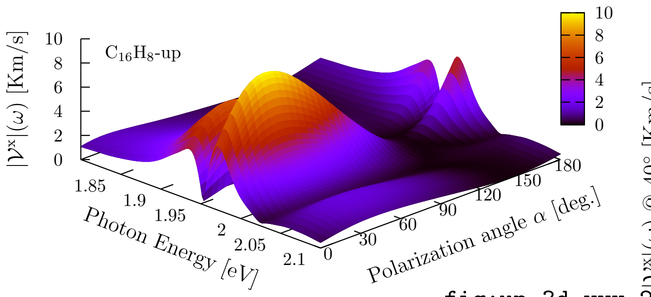
C. Fixing velocity

sec:res-fixvel

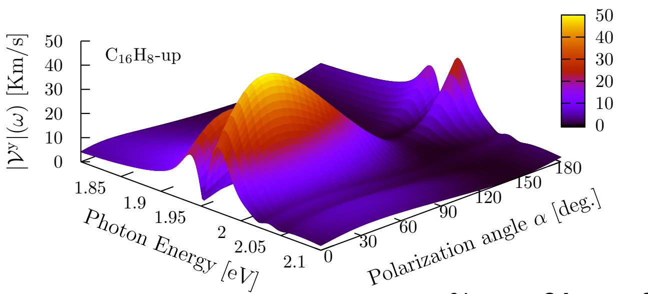
Up structure.

For the *up* structure we first analyzed the energy range from 0.00 eV to 0.16 eV, where we found the most intense response and the absolute maxima for $|\mathcal{V}^{x}|(\omega)$ and $|\mathcal{V}^{y}|(\omega)$ presented in Fig. 8 and resulting from evaluate Eq. (8) using different polarization angles α in Eq. (4) for the *up* structure. ~~We can see that the onset of the response is when the energy of the incoming light is the same of the gap energy.~~ From this picture we can see that for the zone between the energy range of 0.084 eV-0.093 eV and polarization angles between 30° and 45° is the zone where the maximum response is held for both, $|\mathcal{V}^{x}|(\omega)$ and $|\mathcal{V}^{y}|(\omega)$.

In the top frames of Figs. 9(a) and 9(b) we present in solid lines the results of $|\mathcal{V}^{x}|(\omega)$ and $|\mathcal{V}^{y}|(\omega)$, related to the left scale, fixing the polarization angle to $\alpha = 40°$ for which the response is maximized. In the same figures and frames we present in dashed lines the corresponding po-

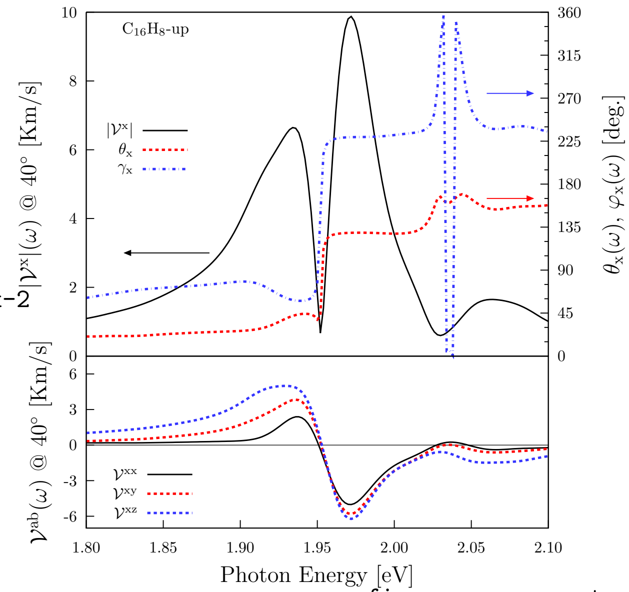


(a) $|\mathcal{V}^{x}|$ for *up* structure fig:up-3d-vvx-2

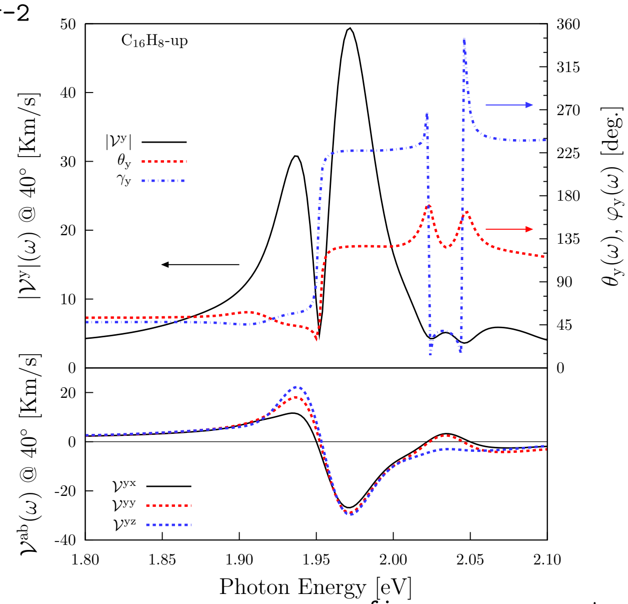


(b) $|\mathcal{V}^{y}|$ for *up* structure fig:up-3d-vvy-2

FIG. 10. $|\mathcal{V}^{a}|(\omega)$ response vs. photon energy vs. polarization angle for the *up* structure. The local maxima of both responses $|\mathcal{V}^{x}|(\omega)$ and $|\mathcal{V}^{y}|(\omega)$ are localized in the energy range from 1.95 eV to 2.00 eV and for polarization angles from 25° to 50°. fig:up-3d-vva-2



(a) $|\mathcal{V}^{x}|$ fig:up-vx-comp-rtp-2



(b) $|\mathcal{V}^{y}|$ fig:up-vy-comp-rtp-2

FIG. 11. Intense response of $|\mathcal{V}^{x}|(\omega)$ and $|\mathcal{V}^{y}|(\omega)$ (top frames left scale of Figs. (a) and (b)), the corresponding polar φ and azimuthal θ angles (top frames right scale), and the corresponding three components (bottom frames) for the *up* structure fixing the polarization angle to $\alpha = 40°$ to maximize the response. fig:up-vab-comp-rtp-2

lar $\theta_a(\omega)$ and azimuthal $\varphi_a(\omega)$ angles related to the right scale. Also, in the bottom frames of those figures we present the decomposition of $|\mathcal{V}^{x}|(\omega)$ and $|\mathcal{V}^{y}|(\omega)$ in the corresponding $\mathcal{V}^{xx}(\omega)$, $\mathcal{V}^{xy}(\omega)$, $\mathcal{V}^{xz}(\omega)$, and $\mathcal{V}^{yx}(\omega)$, $\mathcal{V}^{yy}(\omega)$, $\mathcal{V}^{yz}(\omega)$ components. From Fig. 9(a) we have that for an incoming bean with energy of 0.088 eV the three components have similar contributions and with values of $\mathcal{V}^{xx}(\omega) = -36.5$ Km/s, $\mathcal{V}^{xy}(\omega) = -23.2$ Km/s, and $\mathcal{V}^{xz}(\omega)$ ... 30.8 Km/s resulting in a value of ... being this value the ab... en the spin-velocit... this value corre... angles of $\theta_x(\omega) = 47$... vely, being directed ... upper ... sian Quadrant of the xy plane. Also from this figure we have that those angle values are hold for almost all the peak of the response having a deviation of ±2° in the range of energies from 0.028 eV to 0.098 eV from the corresponding to the absolute maximum mentioned before. Now, from Fig. 9(b) we have that the yx and yy components have less

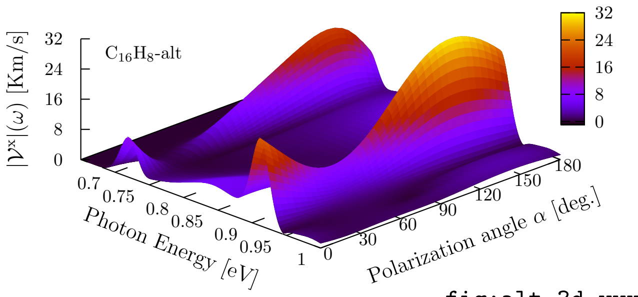
decir que es la direccion hacia donde apunta el espin

contributions for the total response than the yz and for the same incoming beam energy have values of $\mathcal{V}^{yx}(\omega) = -7.9$ Km/s $\mathcal{V}^{yy}(\omega) = 8.6$ Km/s, and $\mathcal{V}^{yz}(\omega) = 87.2$ Km/s resulting in a value of the total response of $|\mathcal{V}^{y}|(\omega) = 87.9$ Km/s being this value the absolute maximum obtained when the spin-velocity is fixed in the y direction and being 1.5 times more intense than $|\mathcal{V}^{\rm x}|(\omega)$ To this absolute maximum correspond spin polar and azimuthal angles $\theta_{\rm y}(\omega) = 8$ and $\varphi_{\rm y}(\omega) = 133$, respectively, being directed almost perpendicularly over the xy plane and being localized on the first Cartesian Quadrant. In a different way than in the $|\mathcal{V}^{\rm x}|(\omega)$ case only the polar angle is hold for the peak of the response having a deviation of $\pm 2^\circ$ since the onset to a energy value of 0.106 eV but the azimuthal angle changes since the onset to 0.106 eV from 99° to 176°. We also found that since the onset of the response till an energy for the incoming beam of 0.118 eV the components of both, $|\mathcal{V}^{\rm x}|(\omega)$ and $|\mathcal{V}^{\rm y}|(\omega)$ have no change in the spin polarization direction. Finally, after this e... value both ... Also there is anot... for an incoming ene... 2.10 eV, correspon... radiation, prese... cal maxima of |... for the *up* struc... that for the zone b... 1.92 eV to 1.94 eV a... and for polarization angl... two local maxima zones are held... the two local maxima are obtained for an energy of the incident beam energies of 1.934 eV and 1.972 eV fixing again the polarization angle to 40°. In the top frames of Figs. 11(a) and 11(b) we present in solid lines the results of $|\mathcal{V}^{\rm x}|(\omega)$ and $|\mathcal{V}^{\rm y}|(\omega)$, related to the left scale, fixing the polarization angle to $\alpha = 40^\circ$ for which the response is maximized for the *up* structure. In the same figures and frames we present in dashed lines the corresponding polar ($\theta_{\rm x}(\omega)$ and $\theta_{\rm y}(\omega)$) and azimuthal ($\varphi_{\rm x}(\omega)$ and $\varphi_{\rm y}(\omega)$) angles related to the right scale. In the bottom frames of same figures we present the decomposition of the responses in the three corresponding components $\mathcal{V}^{\rm xx}(\omega)$, $\mathcal{V}^{\rm xy}(\omega)$, $\mathcal{V}^{\rm xz}(\omega)$ and $\mathcal{V}^{\rm yx}(\omega)$, $\mathcal{V}^{\rm yy}(\omega)$, $\mathcal{V}^{\rm yz}(\omega)$. We found that for both cases, the components have similar contributions and for an incoming energy beam of 1.934 eV we have the first local maximum resulting in a value of $|\mathcal{V}^{\rm x}|(\omega) = 6.6$ Km/s along the x direction with polar and azimuthal spin polarization angles $\theta_{\rm x}(\omega) = 42^\circ$ and $\varphi_{\rm x}(\omega) = 59^\circ$ having fluctuations but being directed over the first Cartesian Quadrant of the xy plane. For the spin moving along the y direction we have a value of $|\mathcal{V}^{\rm y}|(\omega) = 28.7$ Km/s with polar and azimuthal angles $\theta_{\rm y}(\omega) = 45^\circ$ and $\varphi_{\rm y}(\omega) = 56^\circ$ having variations of $\pm 5^\circ$ for energy variations of ± 0.01 eV and being directed over the fir Cartesian Quadrant of the xy plane. Alike, for an incoming energy beam of 1.972 eV we found the second and more intense local maxima with all the components of both responses having similar contributions and resulting in values of $|\mathcal{V}^{\rm x}|(\omega) = 9.9$ Km/s and spin polarization angles $\theta_{\rm x}(\omega) = 129^\circ$ and $\varphi_{\rm x}(\omega) = 229^\circ$ being almost constant in the width of the peak having variations of $\pm 1^\circ$ for variations in energy of ± 0.01 eV and being directed downward the ...d Cartesian Quadrant of the xy plane. For ...g in the y direction we have a ...49.4 Km/s with spin polar- ... 127° and $\varphi_{\rm y}(\omega) = 227^\circ$ ...with variations of $\pm 1^\circ$ ...of ± 1 eV and being di- ...rd Cartesian Quadrant ...ly we have that for bot ...more intense than $|\mathcal{V}^{\rm x}|(\omega)$ ...more intense for 1.932 eV and ...more intense for 1.972 eV. Also all the components of the responses keep the spin polarization positive till an energy of the incoming beam equal to 1.954 eV when the spin polarization changes the direction and after an energy for the incoming beam equal to 2.05 eV both responses goes to zero.

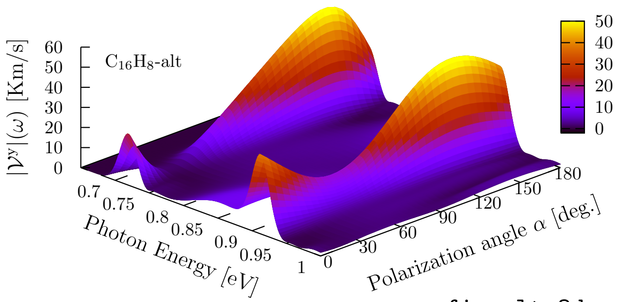
toda la explicacion es confusa y tediosa, ademas se repite en las dos estructuras. Condensa, explica lo más relevante una sola vez, y solo menciona sucintamente los demás resultados. El apache hace que sea dificil de enteder

Alt structure.

For the *alt* structure we analyzed the energy range from 0.6 eV to 1.0 eV, corresponding to the THz radiation, where we found the a local maxima and the most intense responses for $|\mathcal{V}^{\rm x}|(\omega)$ and $|\mathcal{V}^{\rm a}|(\omega)$. In Fig. 12 we present the $|\mathcal{V}^{\rm a}|(\omega)$ spectra resulting from evaluate again Eq. (8) using different polarization angles α in Eq. (4) but now for the *alt* structure. We can see that the onset of the response is when the energy of the incoming light is the same of the gap energy. From this picture we can see that for the zone between the energy range of 0.90 eV-0.93 eV and polarization angles between 120° and 150° is the zone where the maximum response for both, $|\mathcal{V}^{\rm x}|(\omega)$ and $|\mathcal{V}^{\rm y}|(\omega)$ is held. We also found that

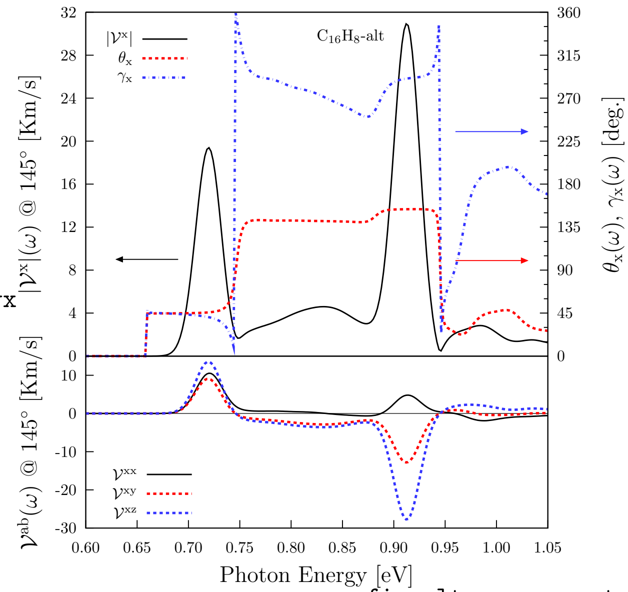


(a) $|\mathcal{V}^{\rm x}|$ for *alt* structure fig:alt-3d-vvx

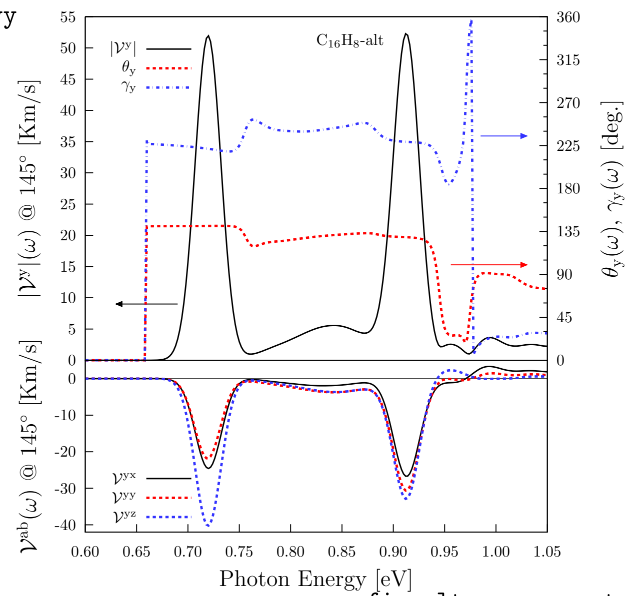


(b) $|\mathcal{V}^{\rm y}|$ for *alt* structure fig:alt-3d-vvy

FIG. 12. $|\mathcal{V}^{\rm a}|(\omega)$ response vs. photon energy vs. polarization angle for the *alt* structure. The absolute maxima of both responses $|\mathcal{V}^{\rm x}|(\omega)$ and $|\mathcal{V}^{\rm y}|(\omega)$ are localized in the energy range from 0.90 eV to 0.93 eV and for polarization angles from 120° to 150°. fig:alt-3d-vva



(a) $|\mathcal{V}^{\rm x}|$ fig:alt-vx-comp-rtp



(b) $|\mathcal{V}^{\rm y}|$ fig:alt-vy-comp-rtp

FIG. 13. Most intense response of $|\mathcal{V}^{\rm x}|(\omega)$ and $|\mathcal{V}^{\rm y}|(\omega)$ (top frames left scale of Figs. (a) and (b)), the corresponding polar φ and azimuthal θ angles (top frames right scale), and the corresponding three components (bottom frames) for the *alt* structure fixing the polarization angle to $\alpha = 145°$ to maximize the response. fig:alt-vab-comp-rtp

the first peak is obtained when the energy of the incoming beam is 0.720 eV and the absolute maximum of the response is obtained when for 0.912 eV, both for a polarization angle $\alpha = 145°$. In the top frames of Figs. 13(a) and 13(b) we present in solid lines the results of $|\mathcal{V}^{\rm x}|(\omega)$ and $|\mathcal{V}^{\rm y}|(\omega)$, related to the left scale, fixing the polarization angle to $\alpha = 145°$ for which the response is maximized for the *alt* structure. In the same figures and frames we present ind dashed lines the spin polarization angles related to the right scale and in the bottom frames the corresponding three components. Making the analysis for the components and angles when the spin current is directed in the x direction, corresponding to the Fig. 13(a), we found that for the *alt* structure when the energy of the incoming beam is 0.720 eV we have similar contributions from all the components resulting in a response of $|\mathcal{V}^{\rm x}|(\omega) = 19.4$ Km/s and polar and azimuthal spin polarization angles $\theta_{\rm x}(\omega) = 46°$ and $\varphi_{\rm x}(\omega) = 41°$ having variations in the range of the peak but being directed over the first Cartesian Quadrant of the xy plane; for an energy of 0.912 eV we have a major contribution from the $\mathcal{V}^{\rm xz}(\omega)$ component resulting in a total response of $|\mathcal{V}^{\rm x}|(\omega) = 30.9$ Km/s and angles $\theta_{\rm x}(\omega) = 154°$, and $\varphi_{\rm x}(\omega) = 290°$ having variations of ±3° in for energy variations of $\pm 1\,\mathrm{eV}$ and being directed downward the fourth Cartesian Quadrant of the xy plane. Making now the analysis for the components and angles when the spin current is directed along the y direction, corresponding to the Fig. 13(b), we found that when the energy of the incoming beam is $0.720\,\mathrm{eV}$ we have more contribution from the $\mathcal{V}^{\mathrm{yz}}(\omega)$ component resulting in a response of $|\mathcal{V}^{\mathrm{y}}|(\omega) = 51.9\,\mathrm{Km/s}$ and angles $\theta_{\mathrm{y}}(\omega) = 141°$ and $\varphi_{\mathrm{y}}(\omega) = 222°$ being the first constant and the second having variations of $\pm 3°$ for energy variations of $\pm 0.3\,\mathrm{eV}$ and being directed downward the third Cartesian Quadrant of the xy plane. Then, for the peak centered at $0.912\,\mathrm{eV}$ we have similar contributions of all the components resulting in a response $|\mathcal{V}^{\mathrm{y}}|(\omega) = 52.3\,\mathrm{Km/s}$ being this the absolute maximum response for the *alt* structure. The corresponding angles are $\theta_{\mathrm{y}}(\omega) = 129°$ and $\varphi_{\mathrm{y}}(\omega) = 229°$ being both constant for the energy range of the peak and being directed downward the third Cartesian Quadrant of the xy plane. Finally we have that the three components of $|\mathcal{V}^{\mathrm{y}}|$ are negative keeping the same spin polarization since the onset of the response to a energy of the incoming beam of $0.886\,\mathrm{eV}$ when the response decreases and goes to zero.

IV. LAYER-BY-LAYER ANALYSIS

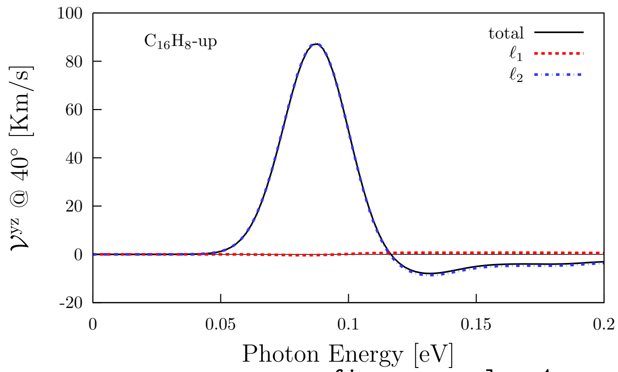
sec:res-layer-by-layer-analysis

motivar para que
hacemos este analis!

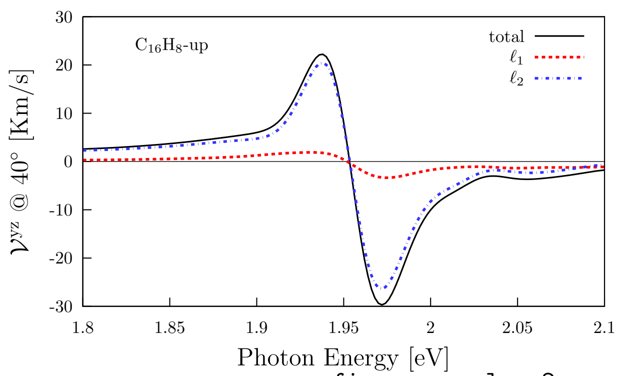
The structures ... into layers to an... tribution for $\mathcal{V}^{\mathrm{ab}}$ ... was divided in six layers corresponding the first one to the top hydrogen atoms, from the second to the forth to carbon atoms in different z positions, and the sixth and last one to the bottom hydrogen atoms. The *up* structure was divid... two layers, the first one com... hydrogen atoms and the s... atoms. The layer divisions ... for the unit cells are shown i...

mejor hay q hacerlo
para V_sigma, pues es
nuestro mejor resultado

From the bottom frames of Figs. 9 and 11 we can see that for the *up* structure again the most intense component of $|\mathcal{V}^{\mathrm{x}}|$ and $|\mathcal{V}^{\mathrm{y}}|$ corresponds to $\mathcal{V}^{\mathrm{yz}}$ which has a value of $87.2\,\mathrm{Km/s}$ for an energy incident beam of $0.088\,\mathrm{eV}$ and $-29.7\,\mathrm{Km/s}$ for an energy incident beam of $1.972\,\mathrm{eV}$. This



(a) fig:up-vyz-lay-1



(b) fig:up-vyz-lay-2

FIG. 14. Layer-by-layer contribution of $\mathcal{V}^{\mathrm{yz}}$ for the *up* structure. fig:up-vyz-lay

component and the corresponding layer by layer contribution is depicted in Fig. 14s. From this figure we have that for the energy range from $0\,\mathrm{eV}$ to $0.2\,\mathrm{eV}$ the response comes from the second layer composed by carbon atoms presented in Tab. II and denoted by the number 2 in Fig. 2. In the other hand, the response for the energy range from $1.8\,\mathrm{eV}$ to $2.1\,\mathrm{eV}$ almost all the response comes from the carbon atoms having a leaser contribution from the hydrogen layer. From the bottom frames of Fig. 13 we can see ... *alt* structure the most intense com... ...nd $|\mathcal{V}^{\mathrm{y}}|$ corresponds to $\mathcal{V}^{\mathrm{yz}}$ which ...40.2 Km/s for an energy incident ...2 eV. This component and the corresponding layer by layer contribution is depicted in Fig. 15. From this figure we have that for the energy range from $0.70\,\mathrm{eV}$ to $0.74\,\mathrm{eV}$ the fifth and sixth layers corresponding to the bottom carbon and hydrogen numbered with 5 and 6 in Fig. 1 have contributions in opposite direction than the other 4 layers resulting in a total response $\mathcal{V}^{yz} = -40.2\,\mathrm{Km/s}$ for an incoming beam energy of $0.72\,\mathrm{eV}$. In the other hand, for the energy range from $0.88\,\mathrm{eV}$ to $0.95\,\mathrm{eV}$ the response for the all six layers the responses are in the same direction resulting in a total response $\mathcal{V}^{yz} = -32.89\,\mathrm{Km/s}$ for an incoming beam with energy of $0.912\,\mathrm{eV}$.

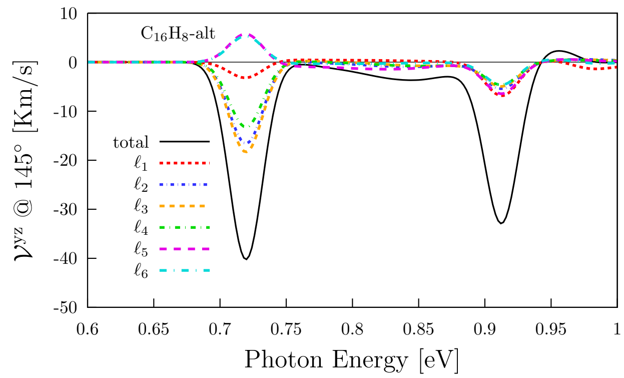


FIG. 15. Layer-by-layer contribution of $\mathcal{V}^{yz}$ for the *alt* structure. `fig:alt-vyz-lay`

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