

# Pure Spin Current Injection in Hydrogenated Graphene Structures

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## I. INTRODUCTION

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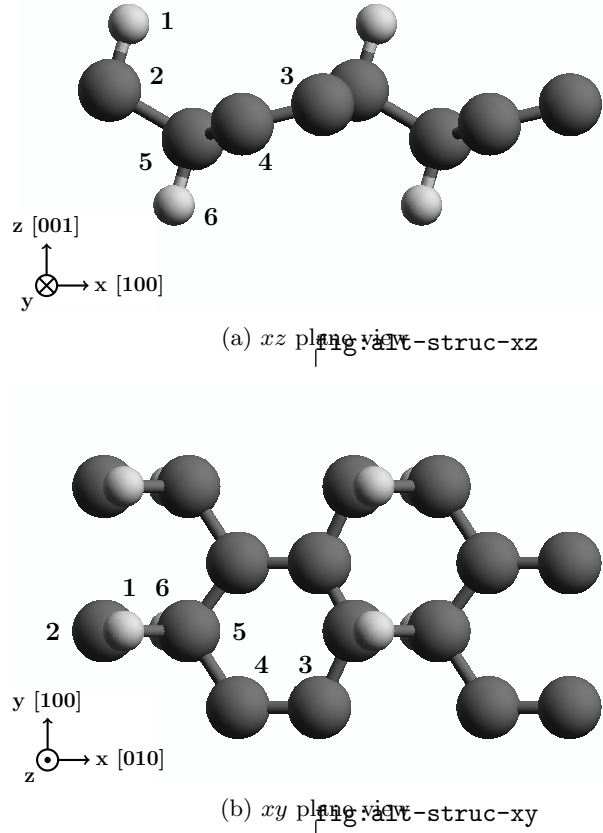


FIG. 1. Alt structure`fig:alt-struc`

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FIG. 2. Up structure `fig:up-struc`

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## II. THEORY

`sec:theory`

The equation for  $\mathcal{V}^{\text{ab}}$  for normal incidence in the *xy* plane with a polarization angle  $\alpha$  is given by

$$\begin{aligned} \mathcal{V}^{\text{ab}}(\omega) &= \frac{2}{\hbar} \frac{\mu^{\text{abxx}}(\omega)E^2(\omega)\cos^2(\alpha) + \mu^{\text{abyy}}(\omega)E^2(\omega)\sin^2(\alpha) + 2\mu^{\text{abxy}}(\omega)E^2(\omega)\cos(\alpha)\sin(\alpha)}{\xi^{\text{xx}}(\omega)E^2(\omega)\cos^2(\alpha) + \xi^{\text{yy}}(\omega)E^2(\omega)\sin^2(\alpha)}, \\ &= \frac{2}{\hbar} \frac{\mu^{\text{abxx}}(\omega)\cos^2(\alpha) + \mu^{\text{abyy}}(\omega)\sin^2(\alpha) + \mu^{\text{abxy}}(\omega)\sin(2\alpha)}{\xi^{\text{xx}}(\omega)\cos^2(\alpha) + \xi^{\text{yy}}(\omega)\sin^2(\alpha)}. \end{aligned} \quad \text{eq:vab} \quad (1)$$

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

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

### A. Fixing velocity.

sec:theory-fixvel

Considering that we have 2D structures we fixed the velocity in the  $xy$  plane along  $x$  and  $y$  directions and we define  $|\mathcal{V}^a|$  as

$$|\mathcal{V}^a| = \sqrt{(\mathcal{V}^{ax})^2 + (\mathcal{V}^{ay})^2 + (\mathcal{V}^{az})^2}, \quad \text{eq:va-mag} \quad (3)$$

and the corresponding polar and azimuthal angles  $\theta$  and  $\varphi$  as

$$\theta = \cos^{-1} \left( \frac{\mathcal{V}^{az}}{|\mathcal{V}^a|} \right), \quad 0 \leq \theta \leq \pi, \quad \text{eq:polar-ang} \quad (4)$$

$$\varphi = \tan^{-1} \left( \frac{\mathcal{V}^{ay}}{\mathcal{V}^{ax}} \right), \quad 0 \leq \varphi \leq 2\pi. \quad \text{eq:azimuthal-ang} \quad (5)$$

### B. Fixing spin

sec:theory-fixspin

In a similar way we can fix in the  $xy$  plane the spin direction along the  $x$ ,  $y$ , and  $z$  directions and then define the magnitude of the spin velocity  $|\mathcal{V}_{\sigma^b}|$  in a fixed angle  $\gamma_b$

$$|\mathcal{V}_{\sigma^b}| = \sqrt{(\mathcal{V}^{ax})^2 + (\mathcal{V}^{ay})^2}, \quad (6)$$

$$\gamma_b = \tan^{-1} \left( \frac{\mathcal{V}^{ay}}{\mathcal{V}^{ax}} \right), \quad (7)$$

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

## III. RESULTS

sec:results

We preset the results for  $\mathcal{V}^{ab}$  for the  $\text{C}_{16}\text{H}_8$ -alt and  $\text{C}_{16}\text{H}_8$ -up structures being 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.

Using the ABINIT code<sup>1</sup> 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-

| Layer No. | Atom type | Position [ $\text{\AA}$ ] |          |          |
|-----------|-----------|---------------------------|----------|----------|
|           |           | $x$                       | $y$      | $z$      |
| 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 [ $\text{\AA}$ ] |          |          |
|-----------|-----------|---------------------------|----------|----------|
|           |           | $x$                       | $y$      | $z$      |
| 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 corresponding layer atom position is depicted in Fig. 2 with the corresponding number of layer.

tab:up-unitcell

Goedecker-Hutter (HGH) relativistic separable dual-space Gaussian pseudopotentials<sup>2</sup> including the spin-orbit interaction for calculating  $\mathcal{V}^a(\omega)$ .

The convergence parameters for the 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  $\mathbf{k}$  points and 8452  $\mathbf{k}$  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. As mentioned in<sup>3</sup>, using DFT the LDA is only one method of many other that can be used to calculate the electronic structure of materials. Also it is known that all methods predict a different band gap than the obtained in the experiment. A correc-

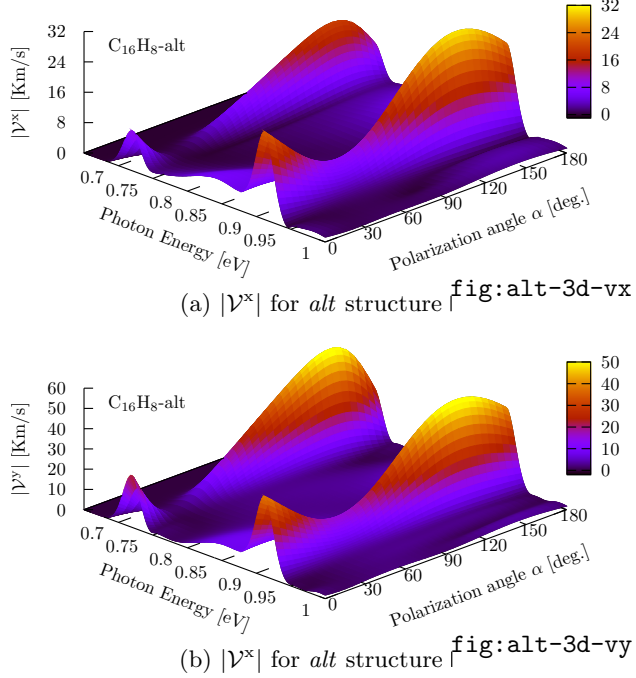


FIG. 3.  $|V^x|$  response for  $C_{16}H_8$ -alt structure. The maximum response zone is localized for an energy range from 0.90 eV to 0.93 eV and for a polarization angle of the incoming beam from  $120^\circ$  to  $150^\circ$ .

tion for the band gap energy value can be calculated by other *ab-initio* methods such as the GW approximation<sup>4</sup> being this outside the scope of this paper.

The structures presented here were divided into layers to analyze the layer-by-layer contribution for  $V^{ab}$  response. The *alt* structure 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 divided into two layers, the first one comprised by the top hydrogen atoms and the second by the carbon atoms. The layer divisions and atom positions for the unit cells are shown in Tables I and II.

### A. Fixing velocity

sec:res-fixvel

#### Alt structure.

For the *alt* structure we analyzed the energy range from 0.6 eV to 1.0 eV where we found the most intense response for  $|V^x|$  and  $|V^y|$ . In Fig.

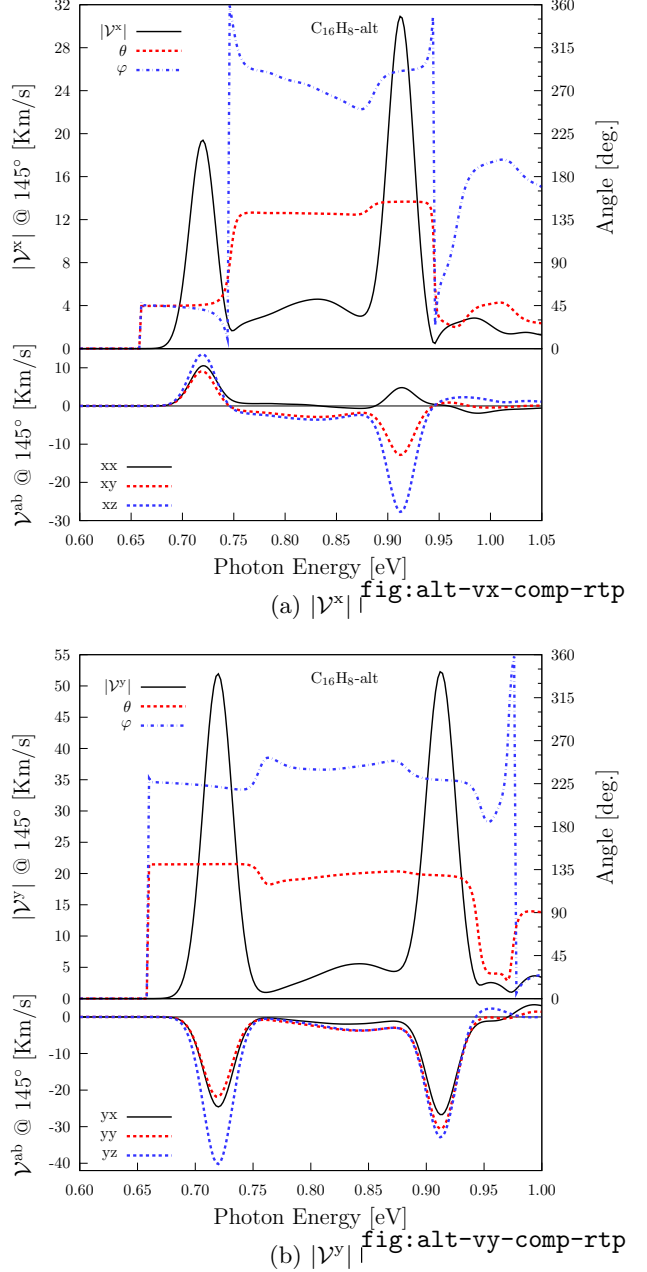


FIG. 4. Most intense responses of  $|V^x|$  and  $|V^y|$  and the corresponding three components for the *alt* structure. Both maxima were obtained for a polarization angle  $\alpha = 145^\circ$ .

fig:alt-vab-comp-rtp

3 we present the  $|V^a|$  spectra resulting from evaluate Eq. (3) using different polarization angles  $\alpha$  in Eq. (1) for the  $C_{16}H_8$ -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  $120^\circ$  and  $150^\circ$  is the zone where the maximum response for both,  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  is kept. We also found that the absolute maximum of the response is obtained when the energy of the incoming beam is 0.912 eV and the polarization angle is  $\alpha = 145^\circ$ . In the top frames of Figs. 4(a) and 4(b) we present the results for  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  (left scale) fixing the polarization angle to  $145^\circ$  for the *alt* structure vs the photon energy and the corresponding polar  $\varphi$  and azimuthal  $\theta$  angles (right scale). Also in the bottom frames of Figs. 4(a) and 4(b) we present the decomposition of  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  in the corresponding components  $\mathcal{V}^{xx}$ ,  $\mathcal{V}^{xy}$ ,  $\mathcal{V}^{xz}$  and  $\mathcal{V}^{yx}$ ,  $\mathcal{V}^{yy}$ ,  $\mathcal{V}^{yz}$  with  $\alpha$  fixed to  $145^\circ$ . Making the analysis for the components and angles for  $|\mathcal{V}^x|$  depicted in Fig. 4(a) we can see that for an incoming beam energy of 0.720 eV the components contributions are similar having values of  $\mathcal{V}^{xx} = 10.5$  Km/s,  $\mathcal{V}^{xy} = 9.1$  Km/s, and  $\mathcal{V}^{xz} = 13.5$  Km/s resulting in a total spin-velocity  $|\mathcal{V}^x| = 19.4$  Km/s and spin polar and azimuthal angles  $\varphi = 45.8^\circ$  and  $\theta = 40.7^\circ$ , respectively. In the other hand, for an energy of the incoming beam equal to 0.912 eV we found that the contribution of the components are  $\mathcal{V}^{xx} = 4.8$  Km/s,  $\mathcal{V}^{xy} = -12.8$  Km/s, and  $\mathcal{V}^{xz} = -27.7$  Km/s having a mayor response coming from the  $xz$  component and resulting in a spin-velocity magnitude  $|\mathcal{V}^x| = 30.9$  Km/s being this the absolute maximum fixing the spin-velocity in the  $x$  direction. Then, the components give us polar and azimuthal angles with values of  $\varphi = 153.8^\circ$  and  $\theta = 290.4^\circ$ . This angles and its variation with the incoming energy beam are presented in the right scale of the top frame of Fig 4(a). Finally we have that since the onset of the response till an energy of the incoming beam of 0.744 eV the three components of  $|\mathcal{V}^x|$  are positive while for the range from 0.746 eV to 0.886 eV the  $\mathcal{V}^{xx}$  component is positive but the  $\mathcal{V}^{xy}$  and  $\mathcal{V}^{xz}$  components change in direction. This is due to a change in the spin polarization direction. Finally after the energy value of 0.886 eV the response decreases and goes to zero. Making now the analysis for  $|\mathcal{V}^y|$  depicted in Fig. 4(b) we have that for an incoming energy beam of 0.720 eV the  $yz$  component have a major contribution than the  $yx$  and  $yy$  com-

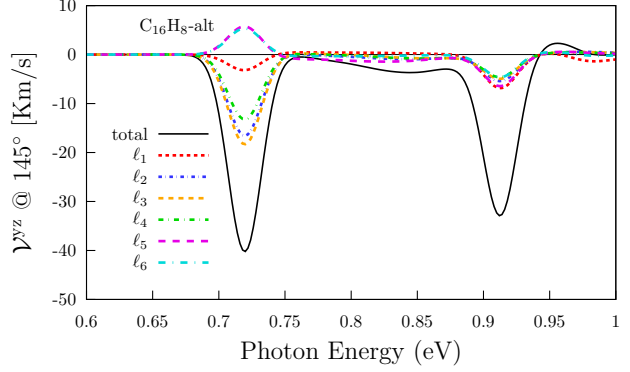


FIG. 5. Layer-by-layer contribution of  $\mathcal{V}^{yz}$  for the *alt* structure. fig:alt-vyz-lay

ponents having values of  $\mathcal{V}^{yx} = -24.6$  Km/s,  $\mathcal{V}^{yy} = -21.8$  Km/s, and  $\mathcal{V}^{yz} = -40.2$  Km/s resulting in a total spin-velocity  $|\mathcal{V}^y| = 51.9$  Km/s and spin polar and azimuthal angles  $\varphi = 140.7^\circ$  and  $\theta = 221.6^\circ$ , respectively. Also, for an energy of the incoming beam of 0.912 eV we found that the contribution of the components are  $\mathcal{V}^{xx} = -26.7$  Km/s,  $\mathcal{V}^{xy} = -30.6$  Km/s, and  $\mathcal{V}^{xz} = -32.9$  Km/s having all the three components similar contributions and resulting in a spin-velocity magnitude  $|\mathcal{V}^y| = 52.3$  Km/s being this the absolute maximum spin-velocity for the velocity fixed to the  $y$  direction and being 1.7 times more intense than the maximum of  $|\mathcal{V}^x|$ . The components then give us the polar and azimuthal angles with values of  $\varphi = 129.0^\circ$  and  $\theta = 228.9^\circ$ , respectively. This angles and the corresponding variation is presented in the right sale of the top frame of Fig. 4(b). We also have that the three components of  $|\mathcal{V}^y|$  are negative keeping the same spin polarization since the onset of the response to a energy of the incoming beam of 0.886 eV when the response decreases and goes to zero. From the bottom frames of Fig. 4 we can see that for the *alt* structure the most intense component of  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  corresponds to  $\mathcal{V}^{yz}$  which has a value of -40.2 Km/s for an energy incident beam of 0.72 eV. This component and the corresponding layer by layer contribution is depicted in Fig. 5. From this figure we have that for the energy range from 0.70 eV to 0.74 eV the fifth and sixth layers corresponding to the bottom carbon and hydrogen numbered with 5 and 6 in Fig. 1 have contributions

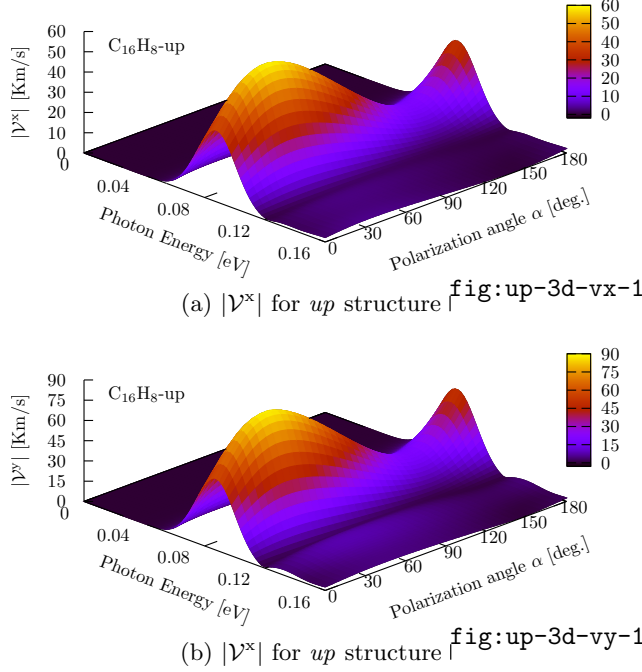


FIG. 6.  $|V^x|$  response for  $C_{16}H_8$ -up structure. The maximum response zone is localized for an energy range from 0.04 eV to 0.12 eV and for a polarization angle of the incoming beam from  $25^\circ$  to  $50^\circ$ .

in opposite direction than the other 4 layers resulting in a total response  $V^{yz} = -40.2$  Km/s for an incoming beam energy of 0.72 eV. In the other hand, for the energy range from 0.88 eV to 0.95 eV the response for the all six layers the responses are in the same direction resulting in a total response  $V^{yz} = -32.89$  Km/s for an incoming beam with energy of 0.912 eV.

#### 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 for  $V^x$  and  $|V^y|$ . In Fig. 6 we present the  $V^a$  spectra resulting from evaluate again Eq. (3) using different polarization angles  $\alpha$  in Eq. (1) but now for the  $C_{16}H_8$ -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  $30^\circ$  and  $45^\circ$  is the zone where the maximum zone of response for both,  $|V^x|$  and  $|V^y|$  is hold. We found that the absolute maximum of the response is obtained when the

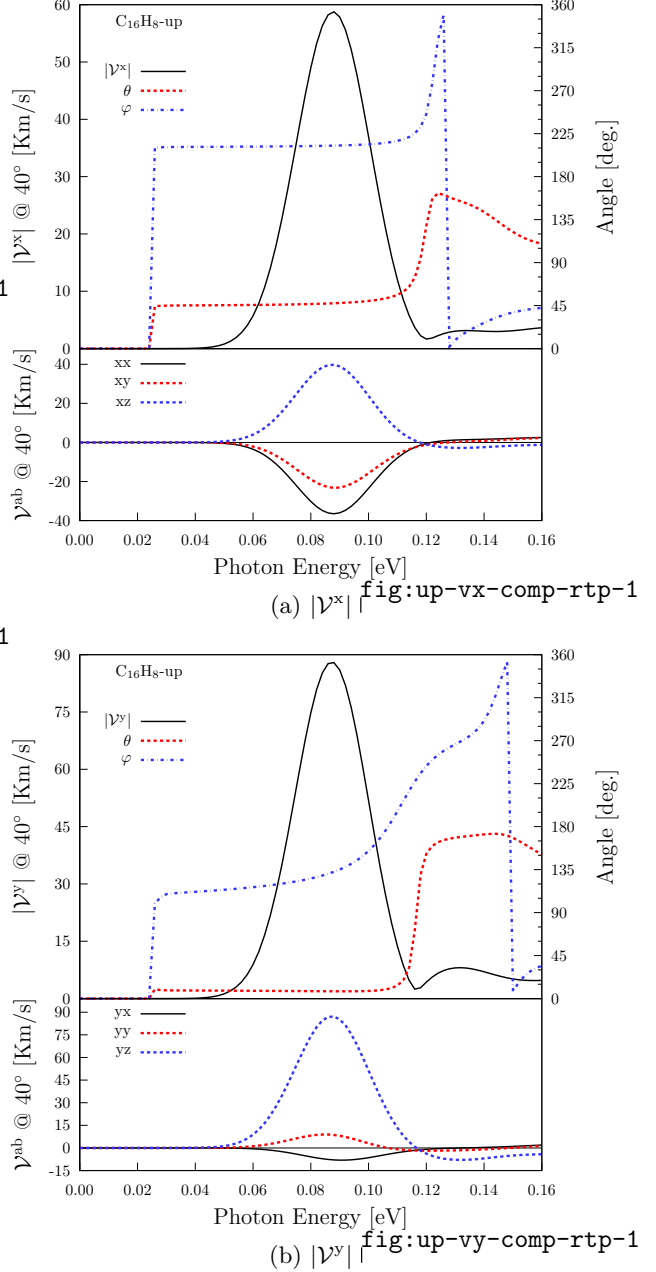


FIG. 7. Most intense responses of  $|V^x|$  and  $|V^y|$  and the corresponding three components for the *up* structure. Both maxima were obtained for a polarization angle  $\alpha = 40^\circ$ .

polarization angle is  $\alpha = 40^\circ$  and the energy of the incoming beam is 0.088 eV. In the top frames of Figs. 7(a) and 7(b) we present the results of  $|V^x|$  and  $|V^y|$  (left scale) fixing the polarization angle to  $\alpha = 40^\circ$  for the *up* structure vs photon energy and the corresponding polar  $\varphi$  and azimuthal  $\theta$  angles (right scale). In the bottom



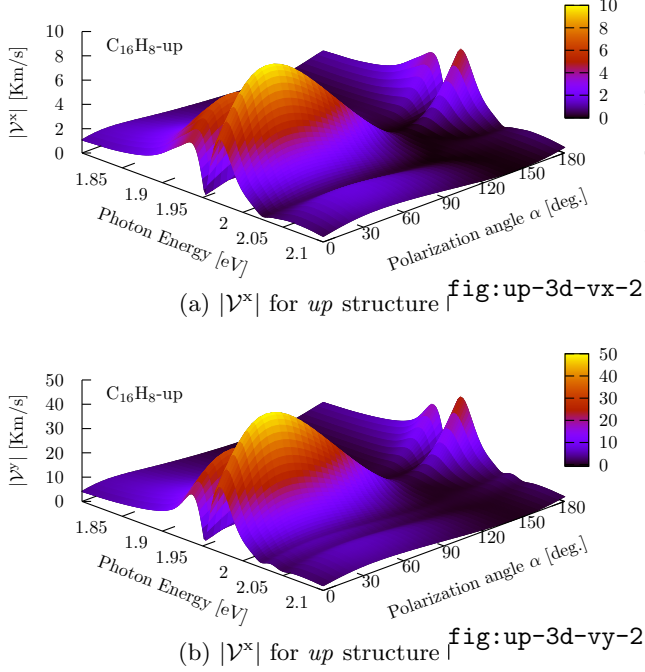


FIG. 8.  $|V^x|$  response for  $C_{16}H_8$ -up structure. The local maximum response zone is localized for an energy range from 1.95 eV to 2.00 eV and for a polarization angle of the incoming beam from 25° to 50°.

frames of same figures we present the decomposition of  $|V^x|$  and  $|V^y|$  in the corresponding  $V^{xx}$ ,  $V^{xy}$ ,  $V^{xz}$ , and  $V^{yx}$ ,  $V^{yy}$ ,  $V^{yz}$  components with  $\alpha$  fixed to 40°.

From Fig. 7(a) we have that for an incoming beam with energy of 0.088 eV the three components have similar contributions and have values of  $V^{xx} = -36.5$  Km/s,  $V^{xy} = -23.2$  Km/s, and  $V^{xz} = 39.8$  Km/s resulting in a value of  $|V^x| = 58.7$  Km/s being this value the absolute maximum obtained when the spin-velocity is fixed in the  $x$  direction. To this value corresponds a polar and azimuthal angles of  $\varphi = 47.4$  and  $\theta = 212.5$ , respectively. Now, from Fig. 7(b) we have that the  $yx$  and  $yy$  components have less contributions for the total response than the  $yz$  and for the same incoming beam energy have values of  $V^{yx} = -7.9$  Km/s,  $V^{yy} = 8.6$  Km/s, and  $V^{yz} = 87.2$  Km/s resulting in a value of the total response of  $|V^y| = 87.9$  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  $|V^x|$  and corresponding spin polar and azimuthal angles  $\varphi = 7.6$

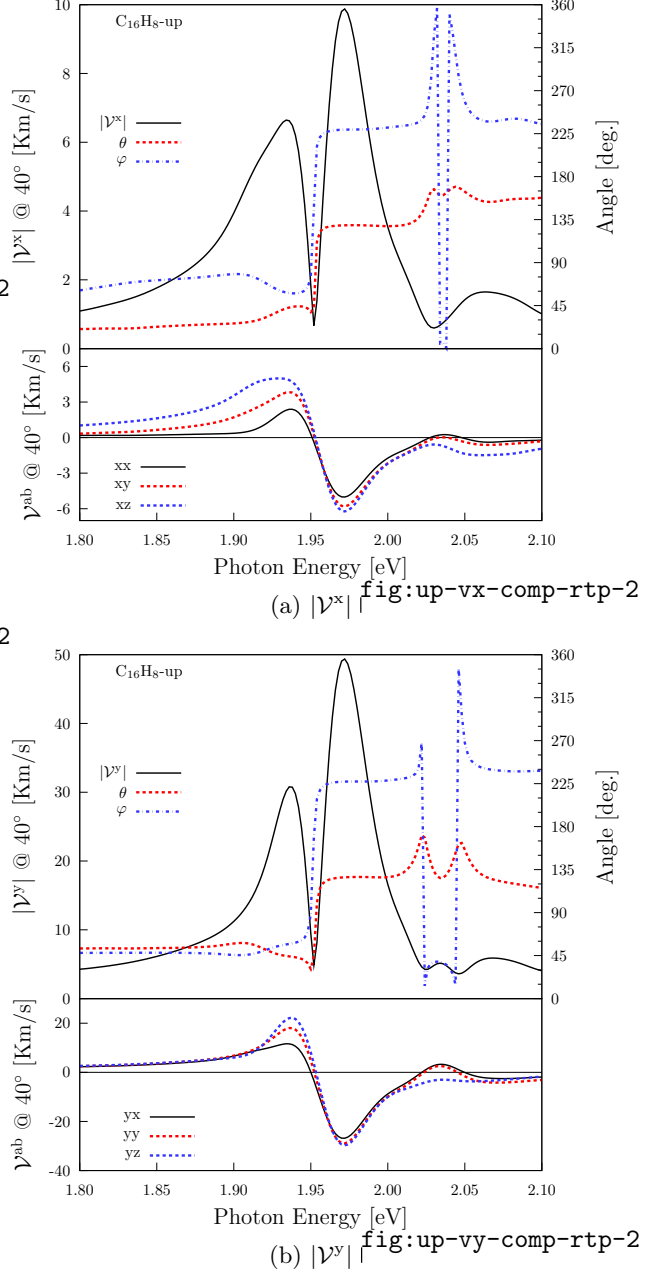


FIG. 9. Intense responses of  $|V^x|$  and  $|V^y|$  and the corresponding three components for the  $up$  structure. Both maxima were obtained for a polarization angle  $\alpha = 40^\circ$ .

$\theta = 132.7$ , respectively. 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,  $|V^x|$  and  $|V^y|$  have no change in the spin polarization direction. Finally, after this energy value both goes to zero. Also there is another energy range of interest for an incoming energy beam from 1.80 eV to 2.10 eV presented

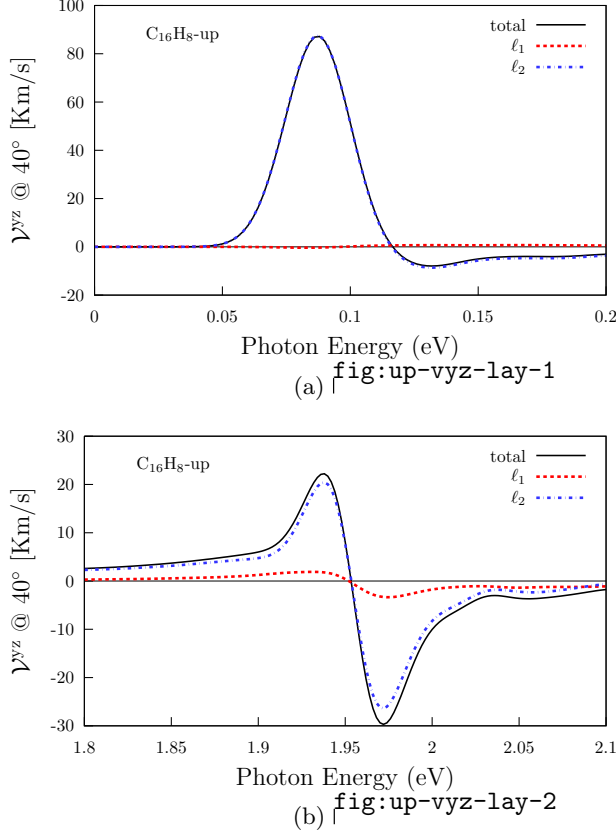


FIG. 10. Layer-by-layer contribution of  $\mathcal{V}^{yz}$  for the *up* structure.

fig:up-vyz-lay

in Fig. 8 where two local maxima of  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  are obtained for the *up* structure resulting from evaluate Eqns. (3) and (1). From this figure we have that for the zone between the energy ranges from 1.92 eV to 1.94 eV and from 1.96 eV to 1.98 eV and angles from  $30^\circ$  to  $45^\circ$  those maxima zones are hold. We found that the maxima are obtained when the polarization angle is fixed to  $40^\circ$  and the corresponding energies are 1.934 eV and 1.972 eV. Again, in the top frames of Figs. 9(a) and 9(b) we present the results of  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  (left scale) fixing the polarization angle to  $\alpha = 40^\circ$  vs the photon energy and the corresponding polar  $\varphi$  and azimuthal  $\theta$  angles (right scale) for the *up* structure. In the bottom frames of same figures we present the three components *xx*, *xy*, *xz*, and *yx*, *yy*, *yz* corresponding to  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  fixing

the polarization angle to  $40^\circ$ . We found that for both cases,  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$ , the corresponding components have similar contributions and for an incoming energy beam of 1.934 eV have values of  $\mathcal{V}^{xx} = 2.3$  Km/s,  $\mathcal{V}^{xy} = 3.8$  Km/s,  $\mathcal{V}^{xz} = 4.9$  Km/s, and  $\mathcal{V}^{yx} = 11.5$  Km/s,  $\mathcal{V}^{yy} = 17.0$  Km/s,  $\mathcal{V}^{yz} = 20.4$  Km/s resulting in a in values of  $|\mathcal{V}^x| = 6.6$  Km/s  $|\mathcal{V}^y| = 28.7$  Km/s being  $|\mathcal{V}^y|$  4.3 times more intense than  $|\mathcal{V}^x|$  for this photon energy. The responses have polar and azimuthal spin polarization angles  $\varphi = 42.0^\circ$  and  $\theta = 58.7^\circ$  for  $|\mathcal{V}^x|$  and  $\varphi = 45.2^\circ$  and  $\theta = 56.0^\circ$  for  $|\mathcal{V}^y|$ . Alike, for an incoming energy beam of 1.972 eV all the components of  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  have similar contributions having values of  $\mathcal{V}^{xx} = -5.0$  Km/s,  $\mathcal{V}^{xy} = -5.8$  Km/s,  $\mathcal{V}^{xz} = -6.2$  Km/s, and  $\mathcal{V}^{yx} = -26.8$  Km/s,  $\mathcal{V}^{yy} = -28.9$  Km/s,  $\mathcal{V}^{yz} = -29.7$  Km/s resulting in a in values of  $|\mathcal{V}^x| = 9.9$  Km/s  $|\mathcal{V}^y| = 49.4$  Km/s being  $|\mathcal{V}^y|$  5.0 times more intense than  $|\mathcal{V}^x|$  for this photon energy. The responses have polar and azimuthal spin polarization angles  $\varphi = 129.0^\circ$   $\theta = 229.1^\circ$  or  $|\mathcal{V}^x|$  and  $\varphi = 127.0^\circ$  and  $\theta = 227.1^\circ$  for  $|\mathcal{V}^y|$ . Finally we have that all the three components of  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  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. From the bottom frames of Figs. 7 and 9 we can see that for the *up* structure again the most intense component of  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$  corresponds to  $\mathcal{V}^{yz}$  which has a value of 87.2 Km/s for an energy incident beam of 0.088 eV and -29.7 Km/s for an energy incident beam of 1.972 eV. This component and the corresponding layer by layer contribution is depicted in Fig. 10s. From this figure we have that for the energy range from 0 eV to 0.2 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 eV to 2.1 eV almost all the response comes from the carbon atoms having a leaser contribution from the hydrogen layer.



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