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Pure Spin Current Injection in Hydrogenated Graphene Structures

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(Dated: April 27, 2017)

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I. INTRODUCTION

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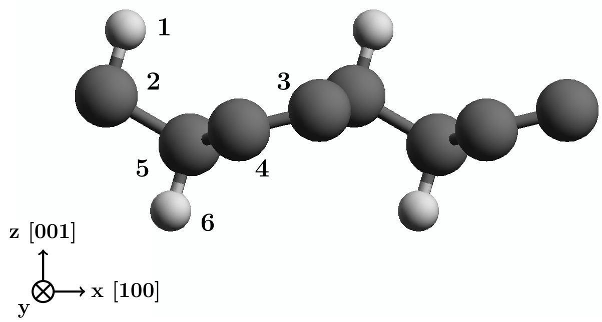
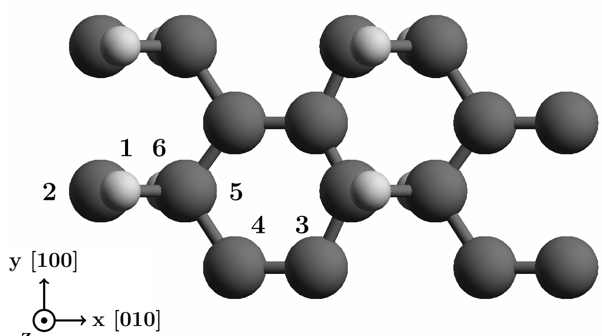


(a) xz plane view fig:alt-struc-xz



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

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

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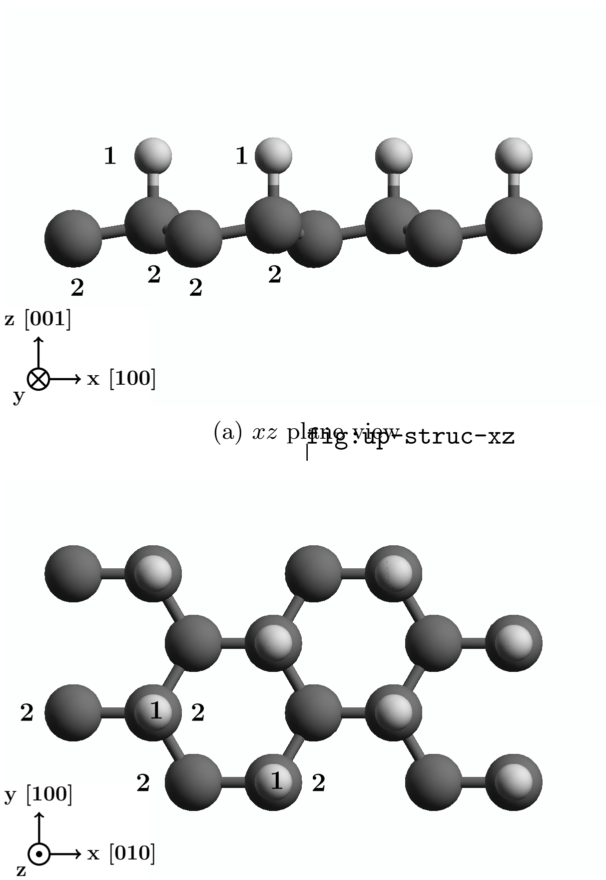

(a) xz plane view fig:up-struc-xz

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

FIG. 2. Up structure fig:up-struc

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II. THEORY

sec:theory

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

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

eq:vab

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

$$\mathcal{V}^{\mathrm{ab}}(\omega) = \frac{2}{\hbar}\frac{\mu^{\mathrm{abxx}}(\omega)+\mu^{\mathrm{abyy}}(\omega)+2\mu^{\mathrm{abxy}}(\omega)}{\xi^{\mathrm{xx}}(\omega)+\xi^{\mathrm{yy}}(\omega)}. \tag{2}$$

eq:vab-90deg

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 $|\mathcal{V}^{\mathrm{a}}|$ as

$$|\mathcal{V}^{\mathrm{a}}| = \sqrt{(\mathcal{V}^{\mathrm{ax}})^2 + (\mathcal{V}^{\mathrm{ay}})^2 + (\mathcal{V}^{\mathrm{az}})^2}, \tag{3}$$

eq:va-mag

and the corresponding polar and azimuthal angles θ and φ as

$$\theta = \cos^{-1}\left(\frac{\mathcal{V}^{\mathrm{az}}}{|\mathcal{V}^{\mathrm{a}}|}\right), \qquad 0 \leq \theta \leq \pi, \tag{4}$$

eq:polar-ang

$$\varphi = \tan^{-1}\left(\frac{\mathcal{V}^{\mathrm{ay}}}{\mathcal{V}^{\mathrm{ax}}}\right), \qquad 0 \leq \varphi \leq 2\pi. \tag{5}$$

eq:azimuthal-ang

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 $|\mathcal{V}_{\sigma^{\mathrm{b}}}|$ in a fixed angle γ_b

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

$$\gamma_{\mathrm{b}} = \tan^{-1}\left(\frac{\mathcal{V}^{\mathrm{ay}}}{\mathcal{V}^{\mathrm{ax}}}\right), \tag{7}$$

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

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 corresponding layer atom position is depicted in Fig. 2 with the corresponding number of layer. tab:up-unitcell

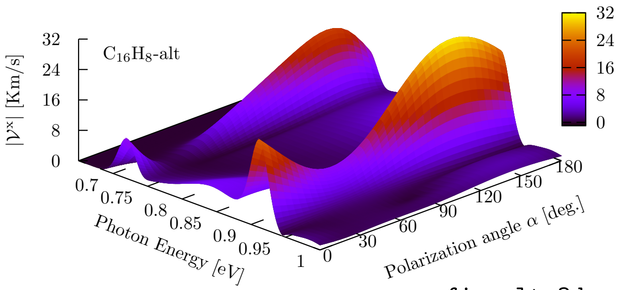
III. RESULTS

sec:results

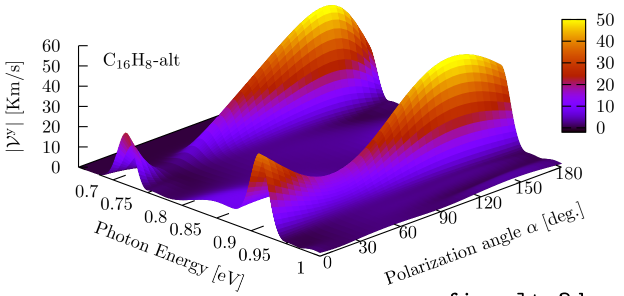
We preset the results for $\mathcal{V}^{\mathrm{ab}}$ for the $C_{16}H_8$-alt and $C_{16}H_8$-up structures being both noncentrosymmetric semi-infinite carbon systems with 50% hydrogenation in different arrangements. The *alt* system has alternating hydrogen atoms on the upper and bottom sides of the 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[1] 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[2] including the spin-orbit interaction for calculating $\mathcal{V}^{\mathrm{a}}(\omega)$.

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 **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. As mentioned in[3], 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-



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



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

FIG. 3. $|\mathcal{V}^{\rm x}|$ 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° to 150°. fig:alt-3d

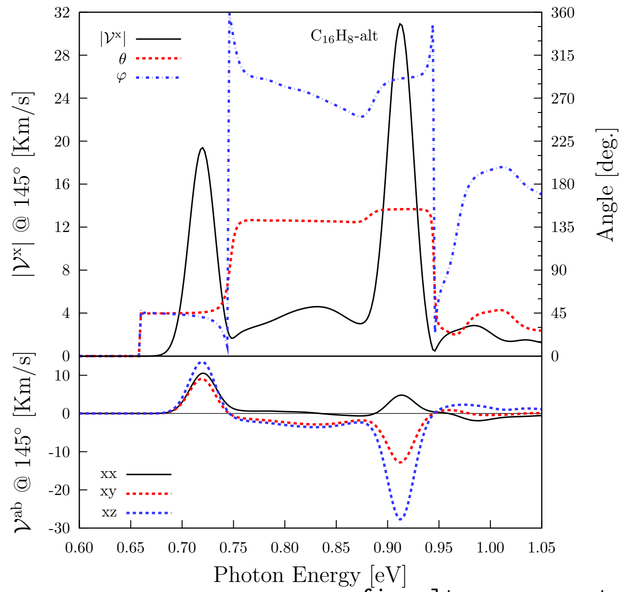
tion for the band gap energy value can be calculated by other *ab-initio* methods such as the GW approximation[4] being this outside the scope of this paper.

The structures presented here where divided into layers to analyze the he layer-by-layer contribution for $\mathcal{V}^{\rm ab}$ 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.

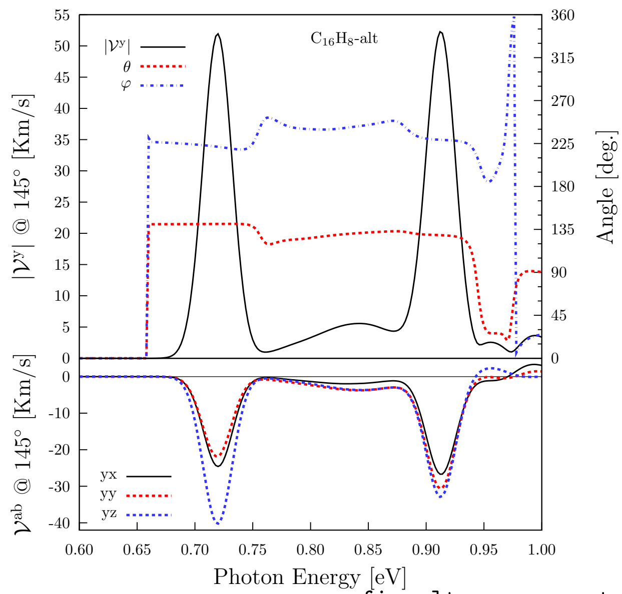
A. Fixing velocity

sec:res-fixvel

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 $|\mathcal{V}^{\rm x}|$ and $|\mathcal{V}^{\rm a}|$. In Fig. 3 we present the $|\mathcal{V}^{\rm a}|$ spectra resulting from evaluate Eq. (3) using different polarization angles α 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



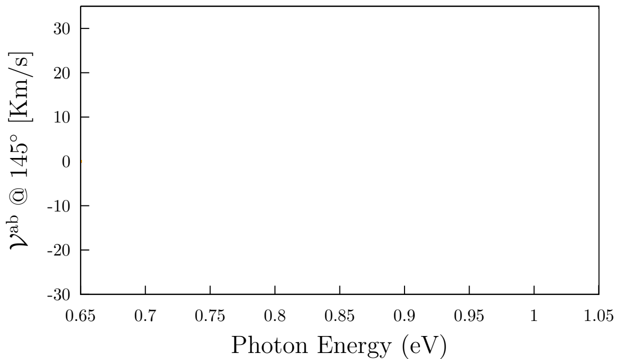
(a) $|\mathcal{V}^{\rm x}|$ fig:alt-vx-comp-rtp



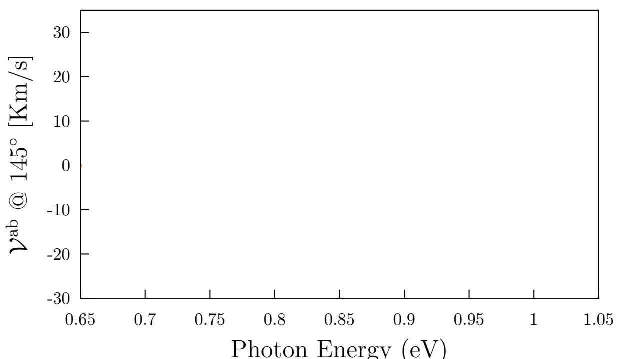
(b) $|\mathcal{V}^{\rm y}|$ fig:alt-vy-comp-rtp

FIG. 4. Most intense responses of $|\mathcal{V}^{\rm x}|$ and $|\mathcal{V}^{\rm y}|$ and the corresponding three components for the *alt* structure. Both maxima where obtained for a polarization angle $\alpha = 145°$. fig:alt-vab-comp-rtp

120° and 150° is the zone where the maximum response for both, $|\mathcal{V}^{\mathrm{x}}|$ and $|\mathcal{V}^{\mathrm{y}}|$ is kept. We also found that the absolute maximum of the response is obtained when the energy of the incoming bean is 0.912 eV and the polarization angle is $\alpha = 145°$. In the top frames of Figs. 4(a) and 4(b) we present the results for $|\mathcal{V}^{\mathrm{x}}|$ and $|\mathcal{V}^{\mathrm{y}}|$ (left scale)fixing the polarization angle to 145° for the *alt* structure vs the photon energy and the corresponding polar φ and azimuthal θ angles (left scale). Also in the bottom frames of Figs. 4(a) and 4(b) we present the decomposition of $|\mathcal{V}^{\mathrm{x}}|$ and $|\mathcal{V}^{\mathrm{y}}|$ in the corresponding components $\mathcal{V}^{\mathrm{xx}}$, $\mathcal{V}^{\mathrm{xy}}$, $\mathcal{V}^{\mathrm{xz}}$ and $\mathcal{V}^{\mathrm{yx}}$, $\mathcal{V}^{\mathrm{yy}}$ $\mathcal{V}^{\mathrm{yz}}$ with α fixed to 145°. Making the analysis for the components and angles for $|\mathcal{V}^{\mathrm{x}}|$ 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 $\mathcal{V}^{\mathrm{xx}} = 10.5\,\mathrm{Km/s}$, $\mathcal{V}^{\mathrm{xy}} = 9.1\,\mathrm{Km/s}$, and $\mathcal{V}^{\mathrm{xz}} = 13.5\,\mathrm{Km/s}$ resulting in a total spin-velocity $|\mathcal{V}^{\mathrm{x}}| = 19.4\,\mathrm{Km/s}$ and spin polar and azimuthal angles $\varphi = 45.8°$ and $\theta = 40.7°$, 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 $\mathcal{V}^{\mathrm{xx}} = 4.8\,\mathrm{Km/s}$ $\mathcal{V}^{\mathrm{xy}} = -12.8\,\mathrm{Km/s}$, and $\mathcal{V}^{\mathrm{xz}} = -27.7\,\mathrm{Km/s}$ having a mayor response coming from the xz component and resulting in a spin- velocity magnitude $|\mathcal{V}^{\mathrm{x}}| = 30.9\,\mathrm{Km/s}$ 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 $\varphi = 153.8°$ and $\theta = 290.4°$. 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 bean of 0.744 eV the three components of $|\mathcal{V}^{\mathrm{x}}|$ are positive while for the range from 0.746 eV to 0.886 eV the $\mathcal{V}^{\mathrm{xx}}$ component is positive but the $\mathcal{V}^{\mathrm{xy}}$ and $\mathcal{V}^{\mathrm{xz}}$ components change in direction. This is due to a change in the spin polarization direction. Finally after the enrgy value of 0.886 eV the response decreases and goes to zero. Making now the analysis for $|\mathcal{V}^{\mathrm{y}}|$ 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 components having values of $\mathcal{V}^{\mathrm{yx}} = -24.6\,\mathrm{Km/s}$, $\mathcal{V}^{\mathrm{yy}} = -21.8\,\mathrm{Km/s}$, and $\mathcal{V}^{\mathrm{yz}} = -40.2\,\mathrm{Km/s}$ resulting in a total spin-velocity $|\mathcal{V}^{\mathrm{y}}| = 51.9\,\mathrm{Km/s}$ and spin polar and azimuthal angles $\varphi = 140.7°$ and $\theta = 221.6°$, respectively. Also, for an energy of the incoming beam of 0.912 eV we found that the contribution of the components are $\mathcal{V}^{\mathrm{xx}} = -26.7\,\mathrm{Km/s}$ $\mathcal{V}^{\mathrm{xy}} = -30.6\,\mathrm{Km/s}$, and $\mathcal{V}^{\mathrm{xz}} = -32.9\,\mathrm{Km/s}$ having all the three components similar contributions and resulting in a spin- velocity magnitude $|\mathcal{V}^{\mathrm{y}}| = 52.3\,\mathrm{Km/s}$ 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 $|\mathcal{V}^{\mathrm{x}}|$. The components then give us the polar and azimuthal angles with values of $\varphi = 129.0°$ and $\theta = 228.9°$, 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 $|\mathcal{V}^{\mathrm{y}}|$ are negative keeping the same spin polarization since the onset of the response to a energy of the incoming beam of 0.886 eV when the response decreases and goes to zero. In Fig. 5 we show the layer-by-layer contribution of $|\mathcal{V}^{\mathrm{ab}}|$ for the *alt* structure. The corresponding layer division and atom types and positions are presented in Table I and depicted in Fig. 1. In the layer- by-layer contribution for $|\mathcal{V}^{\mathrm{x}}|$ (Fig. 5(a)) we have that ... Also, for the layer-by-layer contribution for $|\mathcal{V}^{\mathrm{y}}|$ (Fig. 5(b)) we have that ... From the bottom panels of Fig. 4 we can see that for the *alt* structure 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 -40.21374498 Km/s for an energy incident beam of 0.72 eV. This component and the corresponding layer by layer contribution is depicted in Fig. 6. 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 in opposite direction than the other 4 layers resulting in a total response $\mathcal{V}^{\mathrm{yz}} = -40.2\,\mathrm{Km/s}$ 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 $\mathcal{V}^{\mathrm{yz}} = -32.89\,\mathrm{Km/s}$ for an incoming beam with energy of 0.912 eV.



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



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

FIG. 5. Layer-by-layer contribution of $|\mathcal{V}^{x}|$ and $|\mathcal{V}^{y}|$ for a polarization angle $\alpha = 145°$ for the *alt* structure. fig:alt-vab-lay

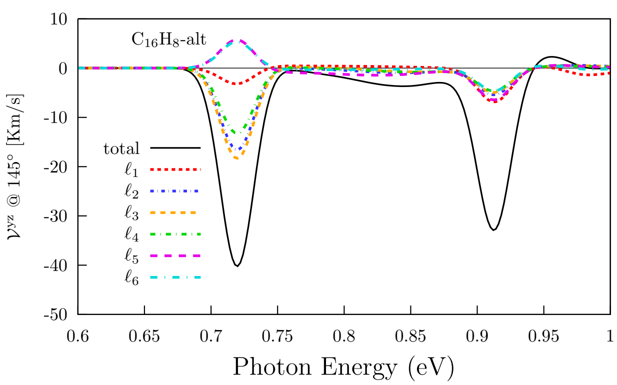
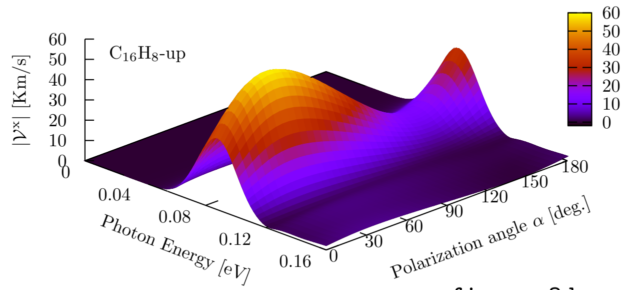
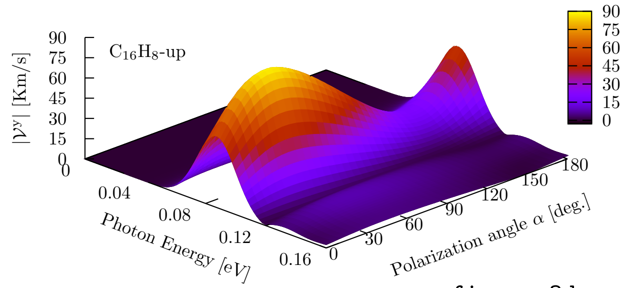


FIG. 6. Layer-by-layer contribution of $\mathcal{V}^{yz}$ for the *alt* structure. fig:alt-vyz-lay



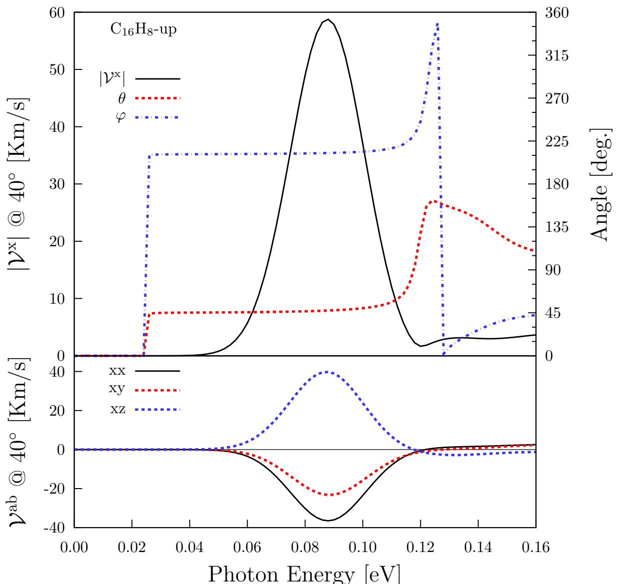
(a) $|\mathcal{V}^{x}|$ for *up* structure fig:up-3d-vx-1



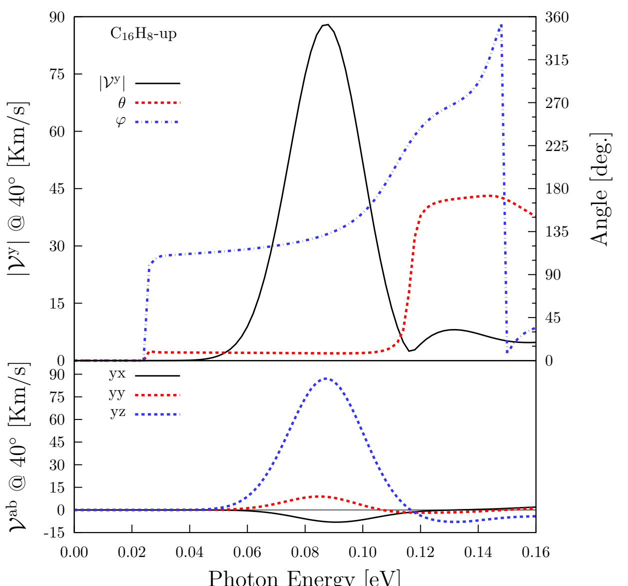
(b) $|\mathcal{V}^{x}|$ for *up* structure fig:up-3d-vy-1

FIG. 7. $|\mathcal{V}^{x}|$ 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° to 50°. fig:up-3d-1

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 $\mathcal{V}^{x}$ and $|\mathcal{V}^{y}|$. In Fig. 7 we present the $\mathcal{V}^{a}$ spectra resulting from evaluate again Eq. (3) using different polarization angles α 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° and 45° is the zone of the maximum response for both, $|\mathcal{V}^{x}|$ and $|\mathcal{V}^{y}|$. We found that the absolute maximum of the response is obtained when the polarization angle is $\alpha = 40°$ and the energy of the incoming beam is 0.088 eV. In Figs. 8(a) and 8(b) we present the results for $|\mathcal{V}^{x}|$ and $|\mathcal{V}^{y}|$ fixing the polarization angle to $\alpha = 40°$ for the *up* structure vs photon energy and the corresponding polar φ and azimuthal θ angles. In the bottom frames of Figs. 8(a) and 8(a) we present the decomposition of $|\mathcal{V}^{x}|$ and $|\mathcal{V}^{y}|$ in the corresponding $\mathcal{V}^{xx}$, $\mathcal{V}^{xy}$, $\mathcal{V}^{xz}$ and $\mathcal{V}^{yx}, \mathcal{V}^{yy}$ $\mathcal{V}^{yz}$ components with α fixed to 40°. From Fig. 8(a) we have that for an incoming bean with energy of 0.088 eV the three components have similar contributions and have values of $\mathcal{V}^{xx} = -36.5$ Km/s, $\mathcal{V}^{xy} = -23.2$ Km/s, and $\mathcal{V}^{xz} = 39.8$ Km/s resulting in a value of $|\mathcal{V}^{x}| = 58.7$ Km/s and corresponding to polar and azimuthal angles of $\varphi = 47.4$ and $\theta = 212.5$, respectively. Now, from Fig. 8(b) we have that



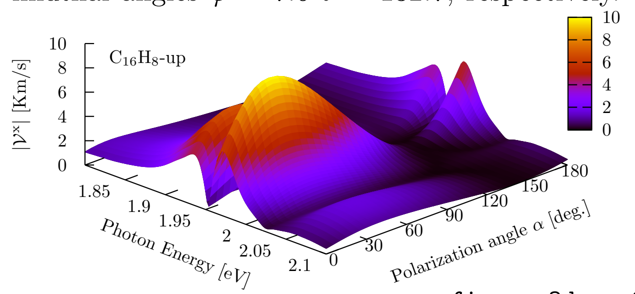
(a) $|\mathcal{V}^{\rm x}|$ fig:up-vx-comp-rtp-1



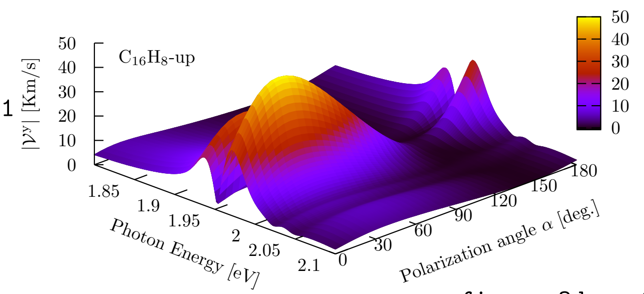
(b) $|\mathcal{V}^{\rm y}|$ fig:up-vy-comp-rtp-1

FIG. 8. Most intense responses of $|\mathcal{V}^{\rm x}|$ and $|\mathcal{V}^{\rm y}|$ and the corresponding three components for the *up* structure. Both maxima where obtained for a polarization angle $\alpha = 40°$. fig:up-vab-comp-rtp-1

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 $\mathcal{V}^{\rm yx} = -7.9\,\text{Km/s}$ $\mathcal{V}^{\rm yy} = 8.5\,\text{Km/s}$, and $\mathcal{V}^{\rm yz} = 87.1\,\text{Km/s}$ resulting in a value of the total response of $|\mathcal{V}^{\rm y}| = 87.9\,\text{Km/s}$ with polar and azimuthal angles $\varphi = 7.6$ $\theta = 132.7$, respectively.



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

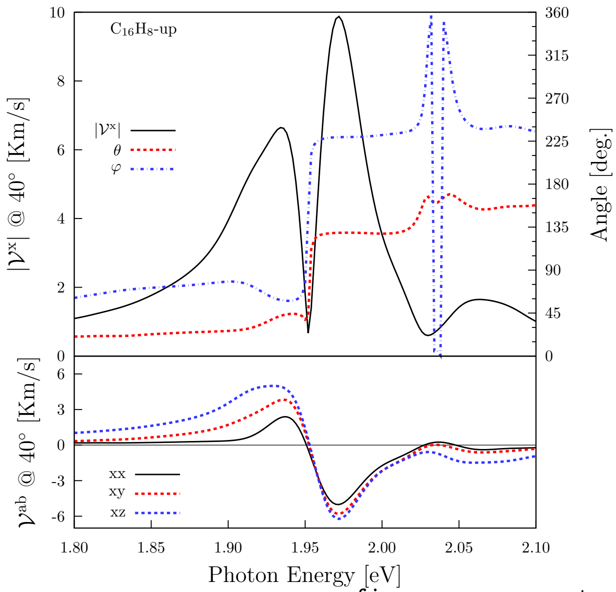


(b) $|\mathcal{V}^{\rm x}|$ for *up* structure fig:up-3d-vy-2

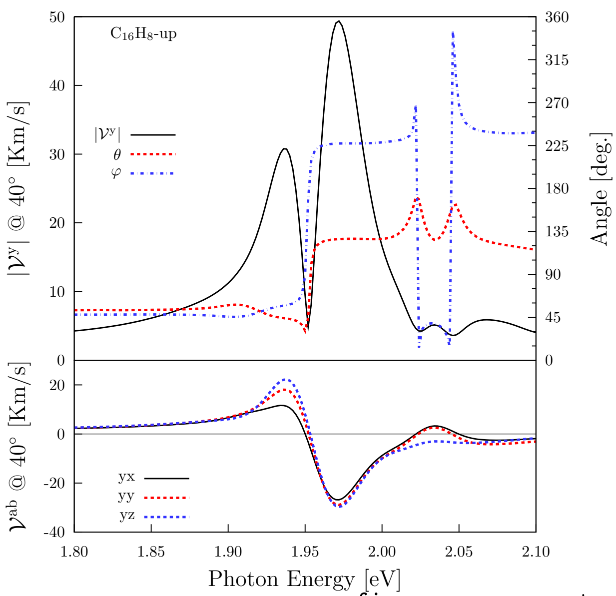
FIG. 9. $|\mathcal{V}^{\rm x}|$ response for $C_{16}H_8$-up structure. The local maximum response zone is localized for an energy range from 1.95 eV to 2.00 eV and for a polarization angle of the incoming beam from 25° to 50°. fig:up-3d-2

Also there is another energy range of interest, from 1.80 eV to 2.10 eV and same polarization angle $\alpha = 40°$ depicted in Fig. 9, where two local maxima are obtained the *up* structure. Again, in the bottom frame of Fig. 10(a) we have the three components $\mathcal{V}^{\rm xx}$, $\mathcal{V}^{\rm xy}$, and $\mathcal{V}^{\rm xz}$ corresponding to $|\mathcal{V}^{\rm x}|$ and in the bottom frame of Fig. 10(b) the three components $\mathcal{V}^{\rm yx}$, $\mathcal{V}^{\rm yy}$, and $\mathcal{V}^{\rm yz}$ corresponding to $|\mathcal{V}^{\rm y}|$ We found that the absolute maximum of the response is obtained when the polarization angle is $\alpha = 40°$. In the top frames of Figs. 8 and 10 we present the results for $|\mathcal{V}^{\rm x}|$ and $|\mathcal{V}^{\rm y}|$ fixing the polarization angle to 40° for the *up* structure vs the photon energy and the corresponding polar φ and azimuthal θ angles for the energy range from 0.0 eV to 0.16 eV and from

[1] X. Gonze, B. Amadon, P.-M. Anglade, J.-M. Beuken, F. Bottin, P. Boulanger, F. Bruneval, D. Caliste, R. Caracas, M. Côté, T. Deutsch,



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



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

FIG. 10. Intense responses of $|\mathcal{V}^{x}|$ and $|\mathcal{V}^{y}|$ and the corresponding three components for the *up* structure. Both maxima where obtained for a polarization angle $\alpha = 40°$. fig:up-vab-comp-rtp-2

L. Genovese, P. Ghosez, M. Giantomassi, S. Goedecker, D. Hamann, P. Hermet, F. Jollet, G. Jomard, S. Leroux, M. Mancini, S. Mazevet, M. Oliveira, G. Onida, Y. Pouillon, T. Rangel, G.-M. Rignanese, D. Sangalli, R. Shaltaf, M. Torrent, M. Verstraete, G. Zerah, and J. Zwanziger, Comput. Phys. Commun. **180**, 2582 (2009).

[2] C. Hartwigsen, S. Goedecker, and J. Hutter, Phys. Rev. B **58**, 3641 (1998).

[3] R. Zapata-Peña, S. M. Anderson, B. S. Mendoza, and A. I. Shkrebtii, physica status solidi (b) **253**, 226 (2016).

[4] G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002). LastBibItem