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Pure Spin Current Injection in Hydrogenated Graphene Structures

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(Dated: April 25, 2017)

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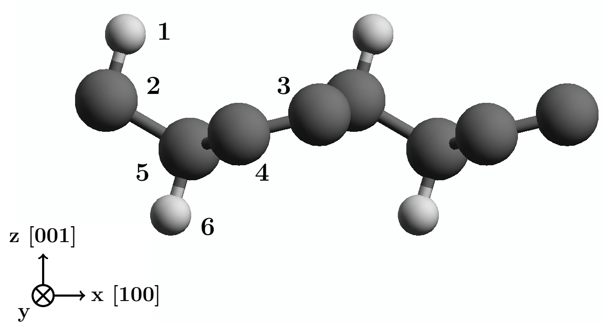
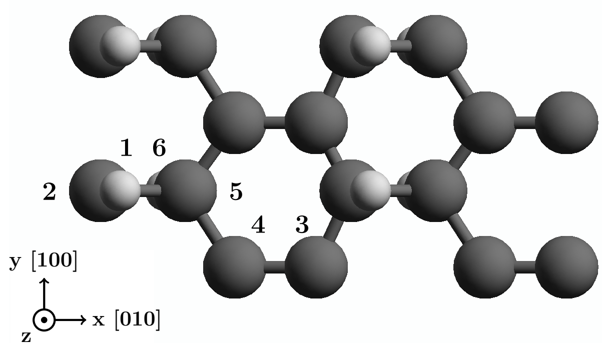
I. INTRODUCTION



(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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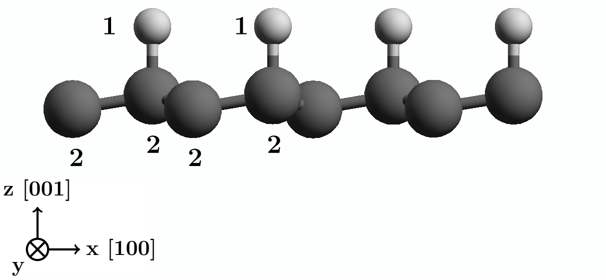
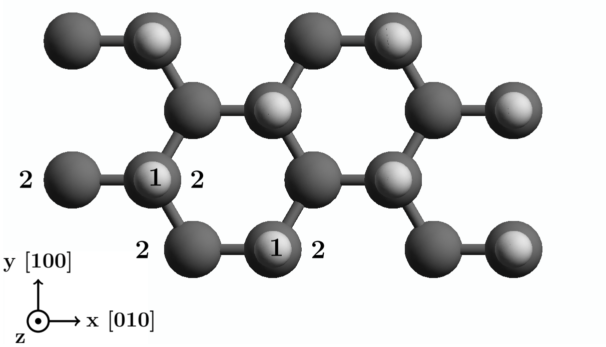


(a) xz plane view fig:up-struc-xz



(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 $|\mathcal{V}^{\rm a}|$ as

eq:va-mag

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

and the corresponding polar and azimuthal angles θ and φ as

eq:polar-ang

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

eq:azimuthal-ang

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

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

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

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

where the angle is measured in the counterclockwise direction from the positive x axis.

III. RESULTS

sec:results

We preset the results for $\mathcal{V}^{\rm ab}$ 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 $\mathcal{V}^{\rm a}(\omega)$.

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

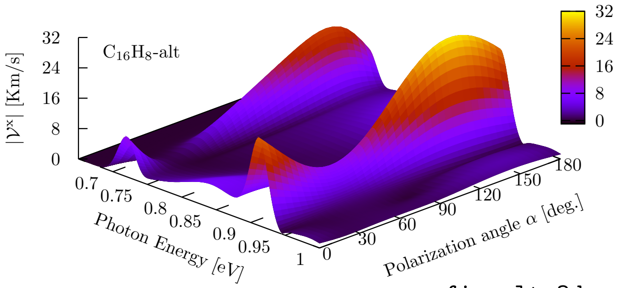
TABLE I. Unit cell of *alt* structure. Layer division, atom types and positions for the *alt* structure. The structure unit cell was divided in six layers corresponding each one to atoms in different z positions. The corresponding layer atom position is depicted in Fig. 1 with the corresponding number of layer. tab:alt-unitcell

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 correction 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.

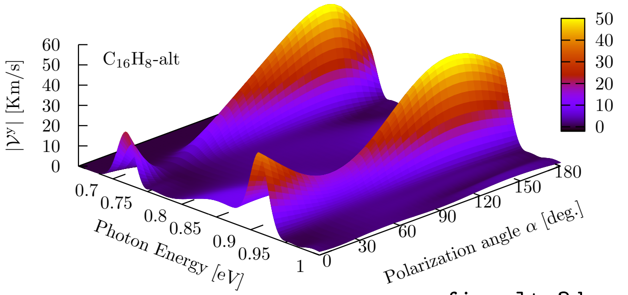
The structures presented here where divided into layers to analyze the he layer-by-layer contribution for $\mathcal{V}^{\rm ab}$ response. The *alt* structure was divided in six layers corresponding the first one to the top hydrogen atoms, from the second to the forth to carbon atoms in different z positions, 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

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`



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



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

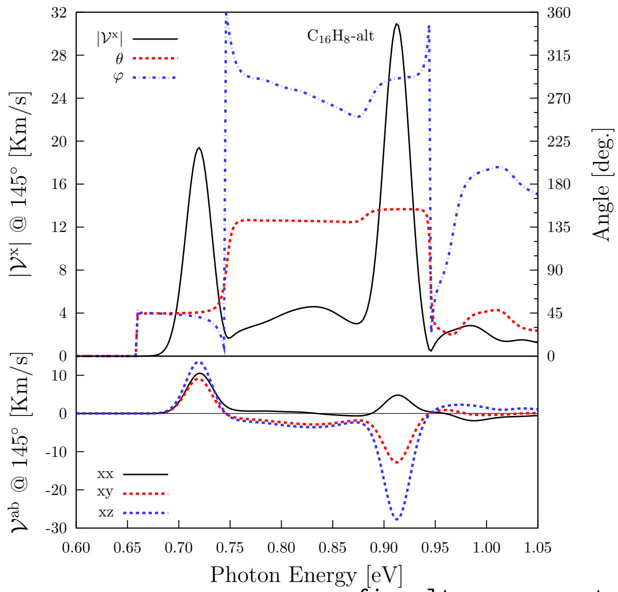
FIG. 3. $|\mathcal{V}^x|$ response for $C_{16}H_8$-alt structure. The maximum response zone is localized for an energy range from 0.90 eV to 0.93 eV. 145° and for a polarization angle of the incoming beam from 120° to 150°. `fig:alt-vab-mag`

for the unit cells are shown in Tables I and II.

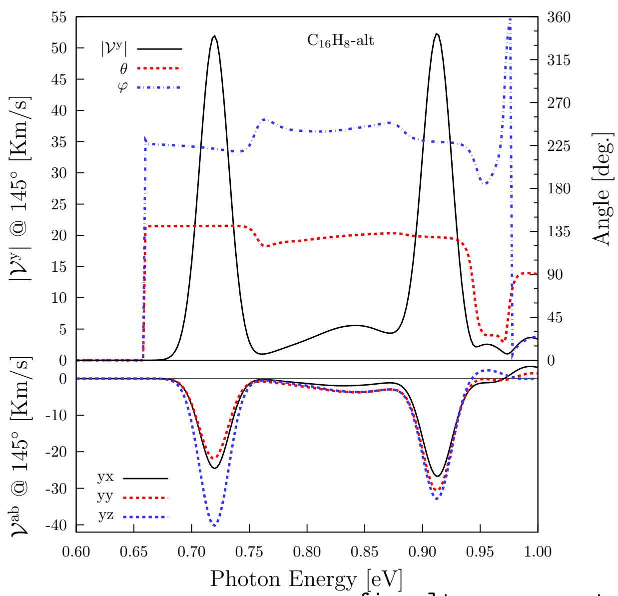
A. Fixing velocity

`sec:res-fixvel`

For the *alt* structure we analyzed the energy range of energy from 0.6 eV to 1.0 eV where we found the most intense response for $\mathcal{V}^{ab}$ and $|\mathcal{V}^a|$.



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



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

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

In Fig. 3 we present the $|\mathcal{V}^a|$ 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 120° and 150° is the zone of the absolute maximum response for both, $|\mathcal{V}^{\mathrm{x}}|$ and $|\mathcal{V}^{\mathrm{y}}|$. Also there is another zone of interest for energies from 0.70 eV to 0.74 eV where a local maximum is obtained. From Fig. 3(a) we have that $|\mathcal{V}^{\mathrm{x}}|$reaches values of 30 Km/s for the first zone mentioned before and 20 Km/s for the second one. We also found that the absolute maximum of the response is obtained when 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 $|\mathcal{V}^{\mathrm{y}}|$ fixing the polarization angle to 145° for the *alt* structure vs the photon energy and the corresponding azimuthal θ and polar φ angles. 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 $\mathcal{V}^{\mathrm{xx}}$, $\mathcal{V}^{\mathrm{xy}}$, $\mathcal{V}^{\mathrm{xz}}$ and $\mathcal{V}^{\mathrm{yx}}$,$\mathcal{V}^{\mathrm{yy}}$ $\mathcal{V}^{\mathrm{yz}}$ components for the fixed polarization angle. Making the analysis for the components and angles for $|\mathcal{V}^{\mathrm{x}}|$ we can see that for the energy range from 0.70 eV to 0.74 eV all the xx, xy, and xz components contribute with almost the same intensity giving a total spin-velocity of 19.3 Km/s and spin polar and azimuthal angles $\varphi = 45.8°$ and $\theta = 40.7°$. In the other hand, for the energy range from 0.88 eV to 0.95 eV there is a major contribution coming from the $\mathcal{V}^{\mathrm{xz}}$ component resulting in a spin-velocity magnitude of 30.9 Km/s being this magnitude the most intense for $|\mathcal{V}^{\mathrm{x}}|$. In this case the polar angle is $\varphi = 153.8°$ and the spin angle over the xy plane have is $\theta = 290.4°$. Also we notice that for the range of 0.70-0.74 eV all the contributions are positive while for the range of 0.88-0.95 eV the xx component remains positive but the components xy and xz change in direction. This is due to a change in the spin polarization. Making now the analysis for $|\mathcal{V}^{\mathrm{y}}|$ we have that for the energy range from 0.70 eV to 0.74 eV the yz component have a more intense response than yx and yy components and they give a total spin-velocity of 51.9 Km/s and result in polar angle $\varphi = 140.7°$ and spin azimuthal angle of $\theta = 221.5°$. For the energy range from 0.88 eV to 0.95 eV all three components have similar intensities resulting in a spin-velocity magnitude of $|\mathcal{V}^{\mathrm{y}}| = 52.3$ Km/s being this response 1.7 times mores intense than the most intense response of $|\mathcal{V}^{\mathrm{x}}|$. The corresponding polar and azimuthal angles for $|\mathcal{V}^{\mathrm{y}}|$ in this energy range are $\theta = 129.0°$ and $\varphi = 228.9°$. Now we have that the three components of $|\mathcal{V}^{\mathrm{y}}|$ are negative for the energy range from 0.60 eV to 1.0 eV keeping the same spin polarization for all this range.

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[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