

# Pure Spin Current Injection in Hydrogenated Graphene Structures

Reinaldo Zapata-Peña, Bernardo S. Mendoza, Anatoli I. Shkrebti

## 1 Introuction

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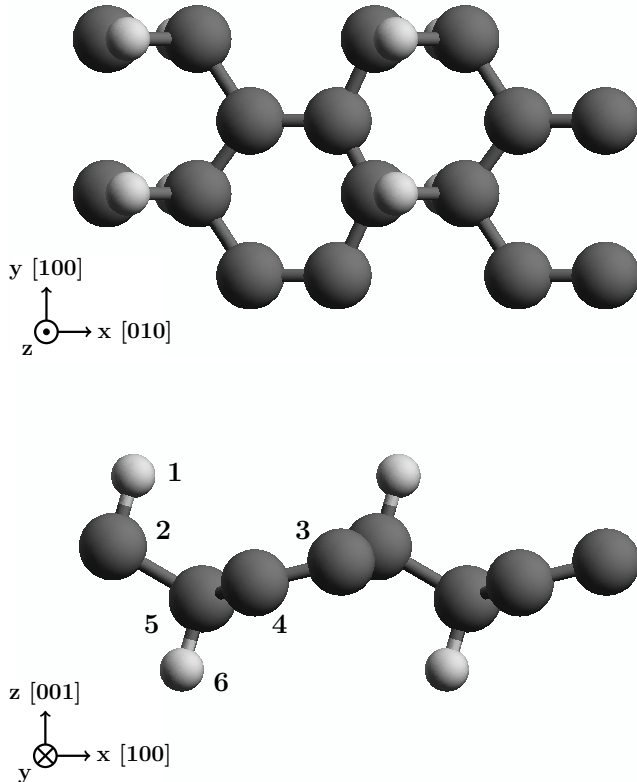


Figure 1: Alt structure.

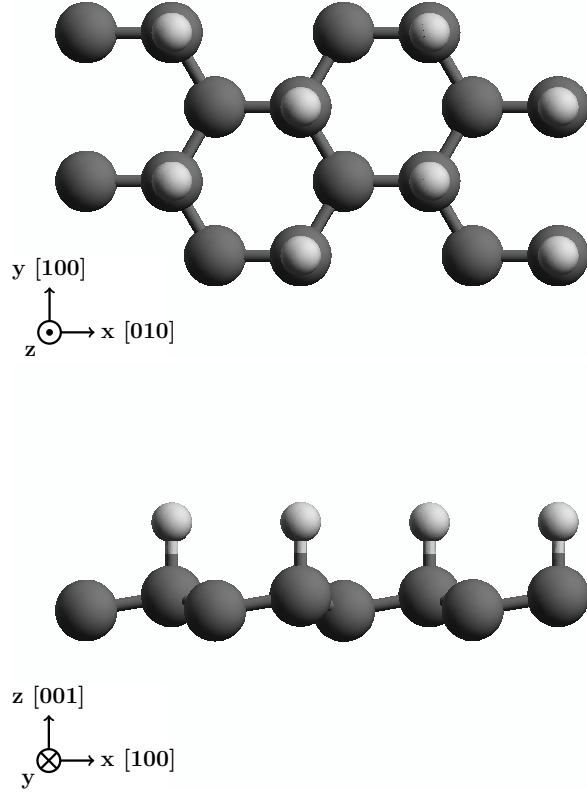


Figure 2: Up structure

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## 2 Theory

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

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

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

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

We also define  $|\mathcal{V}^{\text{a}}|$  as

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

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

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

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

(6)

## 3 Results

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

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 [4], 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 [3] being this outside the scope of this paper.

The structures presented here were divided into layers to analyze the layer-by-layer contribution for  $\mathcal{V}^{\text{ab}}$  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 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 1: 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.

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 2: 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.

### 3.1 alt

In Fig. 3 we present the  $\mathcal{V}^x$  spectra resulting from evaluate the Eq. (3) at using different polarization angles  $\alpha$  in Eq. (1) for the  $C_{16}H_8$ -alt structure. 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 maximum response is held reaching values of  $\mathcal{V}^x$  near to 30 Km/s. Also there is a second zone between the energy range of 0.70 eV-0.74 eV and same polarization angles where a local maximum of  $\mathcal{V}^x$  reaching values near to 22 Km/s. We also found that the absolute maximum of the response is obtained for a polarization angle  $\alpha = 145^\circ$ . The decomposition of  $|\mathcal{V}^a|$  in the corresponding  $\mathcal{V}^x$ ,  $\mathcal{V}^y$ , and  $\mathcal{V}^z$  components is depicted in Fig. 4. From this figure we can see that for the energy range from 0.70 eV to 0.74 eV all the  $x$ ,  $y$ , and  $z$  components contribute with almost the same intensity. In the other hand, for the energy range from 0.88 eV to 0.95 eV there is a major contribution coming from the  $\mathcal{V}^{xz}$  component.

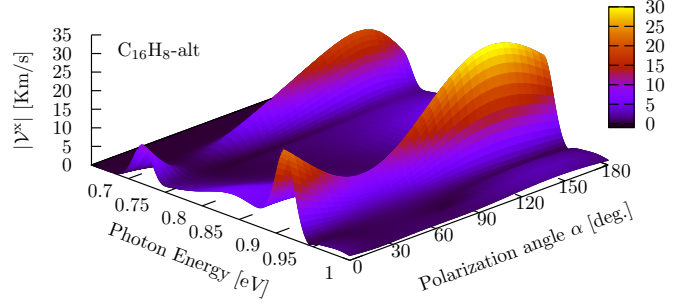


Figure 3:  $\mathcal{V}^x$  for  $C_{16}H_8$ -alt structure. The maximum response zone is localized for an energy range from 0.90 eV to 0.93 eV, 145° and for a polarization angle of the incoming beam from 120° to 150°.

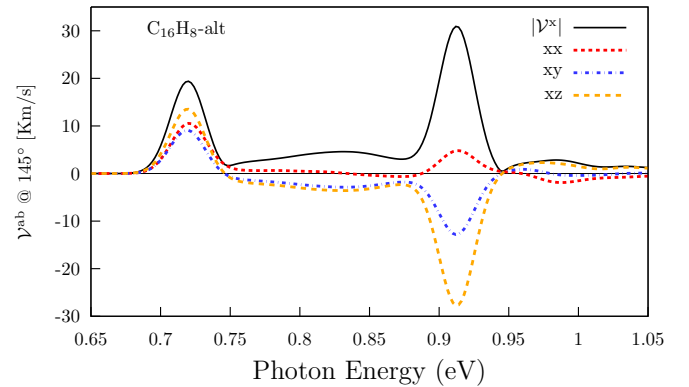


Figure 4: Three components of  $\mathcal{V}^x$  @ 145°.

### 3.1.1 $\nu^y$

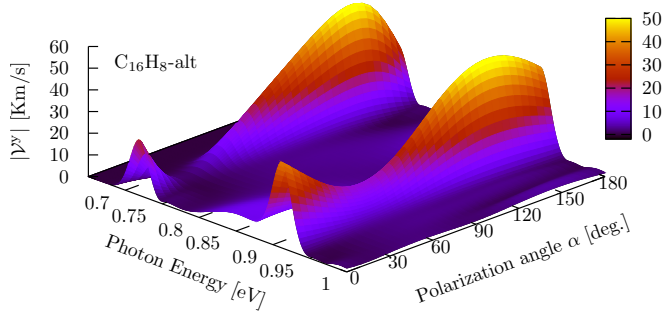


Figure 5: The most intense response for  $\nu^y$  is for  $145^\circ$ .

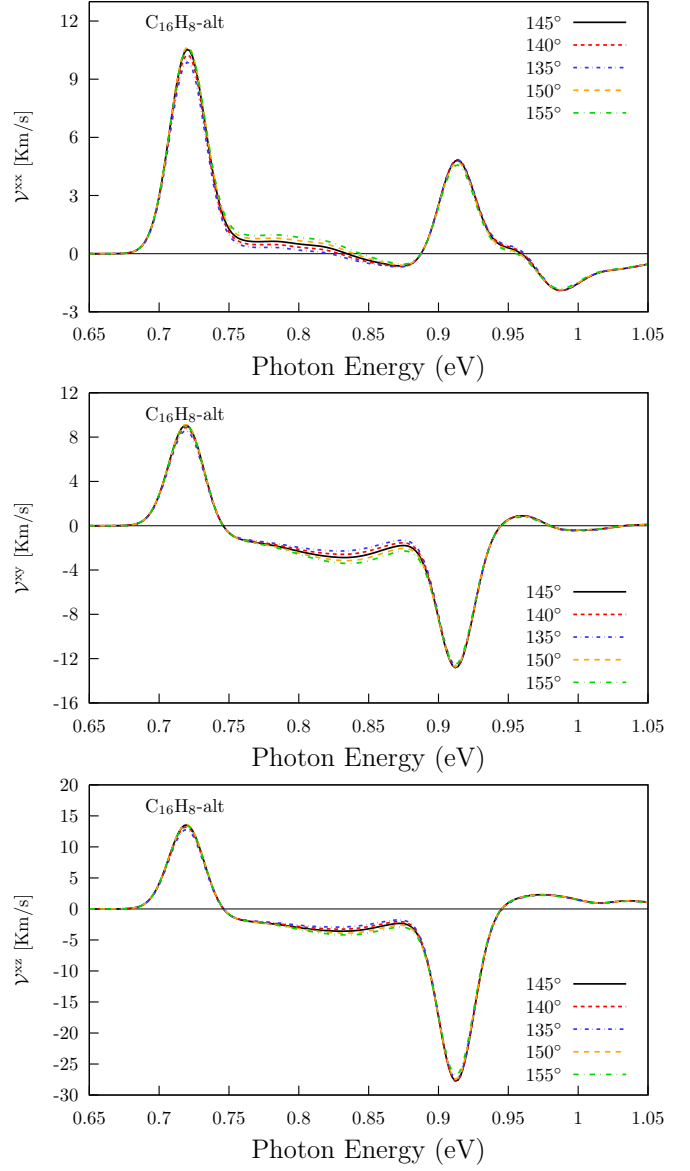


Figure 6: Cheking angle of incidence for  $yb$  components.

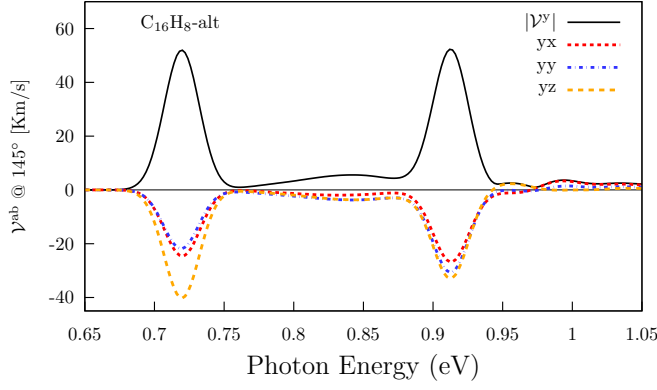


Figure 7: Three components of  $\mathcal{V}^y$  @  $145^\circ$ .

### 3.1.2 $|\mathcal{V}^{ab}|$ , angles $\theta$ and $\varphi$ , layers, and comparison with CdSe and GaAs.

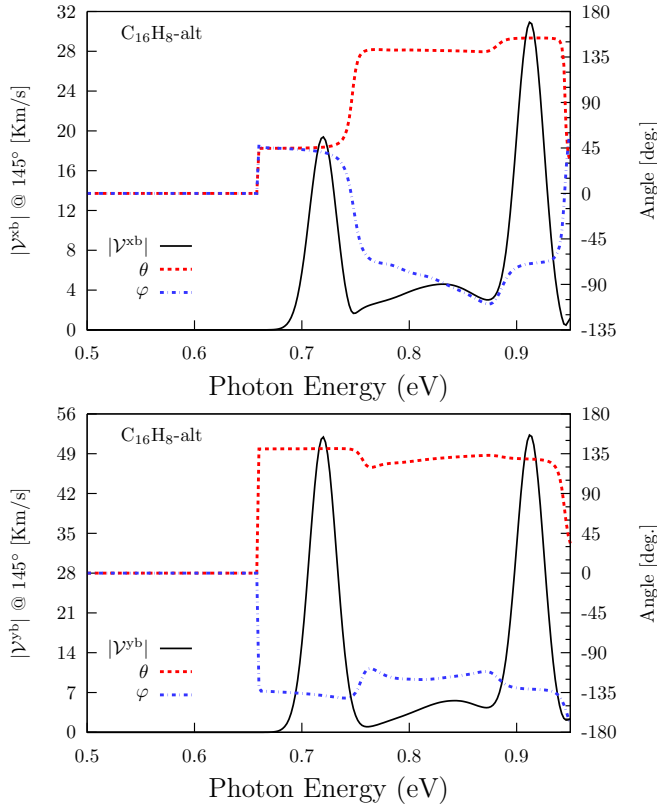


Figure 8:  $|\mathcal{V}^{ab}|$  (solid line, leftside scale) and the corresponding angles  $\theta$  and  $\varphi$  (dashed lines, rightside scale).

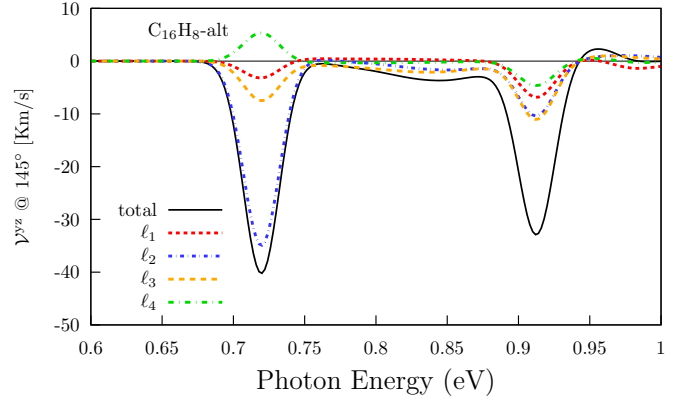


Figure 9: Layer decomposition for the most intense response:  $\mathcal{V}^{yz}$ .

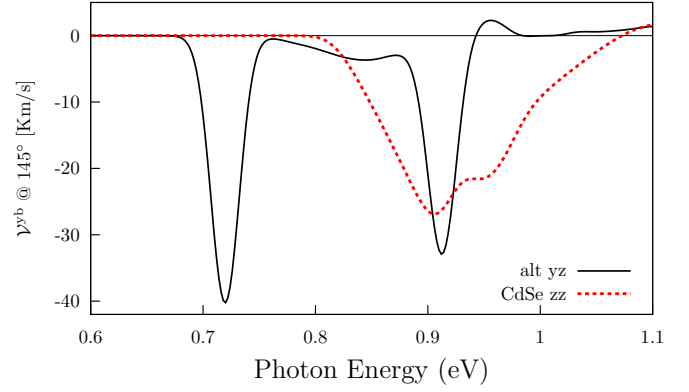


Figure 10: Comparison of the most intense response vs the most intense responses of CdSe and GaAs.

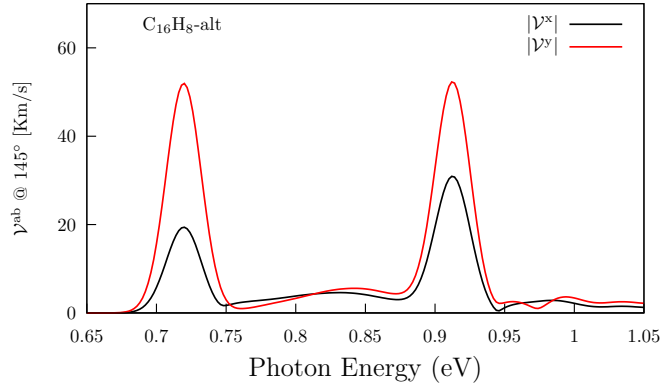


Figure 11: Comparisson of  $|\mathcal{V}^x|$  and  $|\mathcal{V}^y|$

## 3.2 Up (graphone)

### 3.2.1 $\mathcal{V}^x$ energy range 0.0–0.2 eV

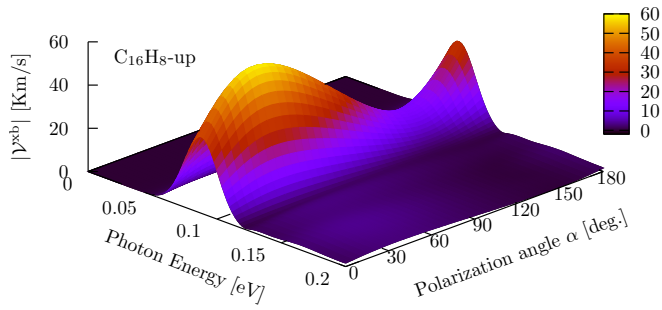


Figure 12: The most intense response for  $\mathcal{V}^x$  is for  $40^\circ$ .

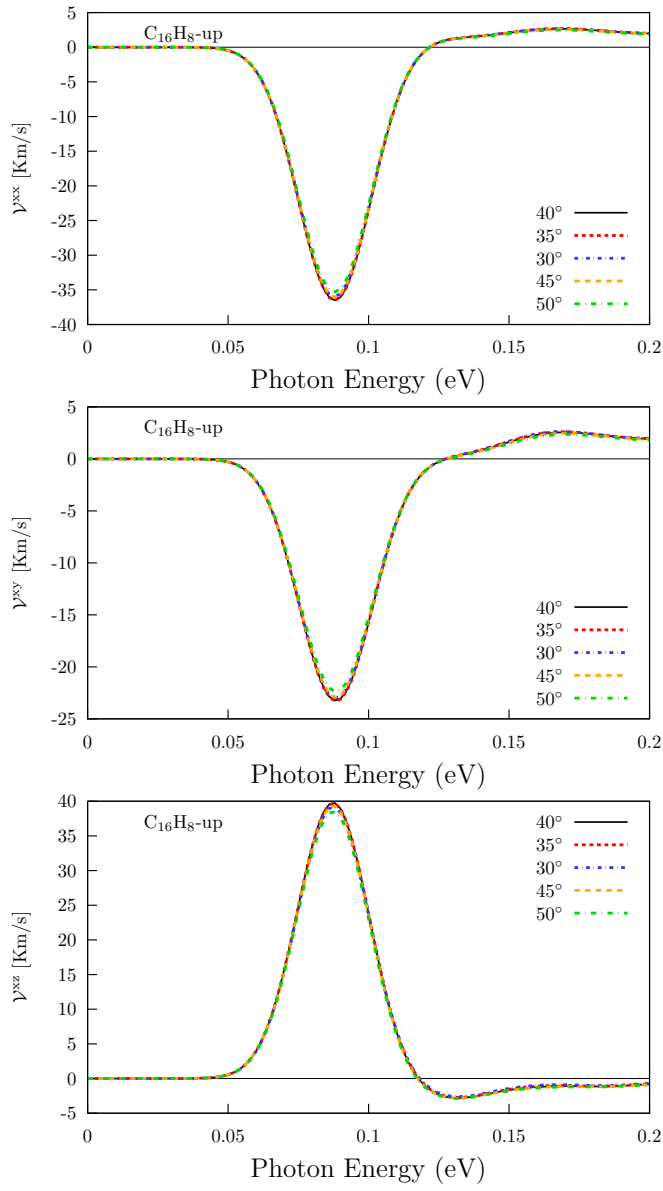


Figure 13: Cheking angle of incidence for  $xb$  components for up structure.

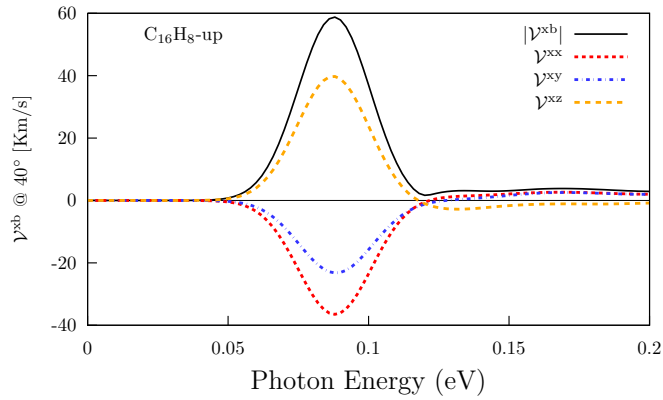


Figure 14: Three components of  $\mathcal{V}^x$  @ 40°.

### 3.2.2 $\mathcal{V}^y$ energy range 0.0–0.2 eV

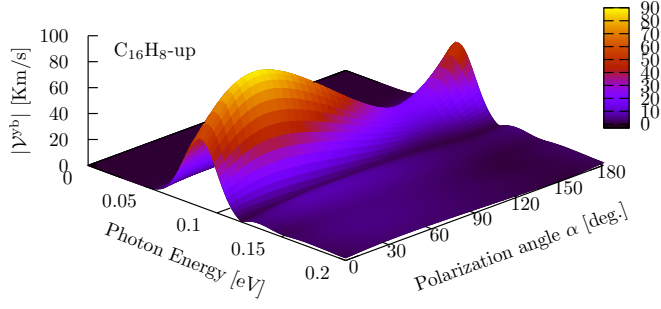


Figure 15: The most intense response for  $\mathcal{V}^y$  is for  $40^\circ$ .

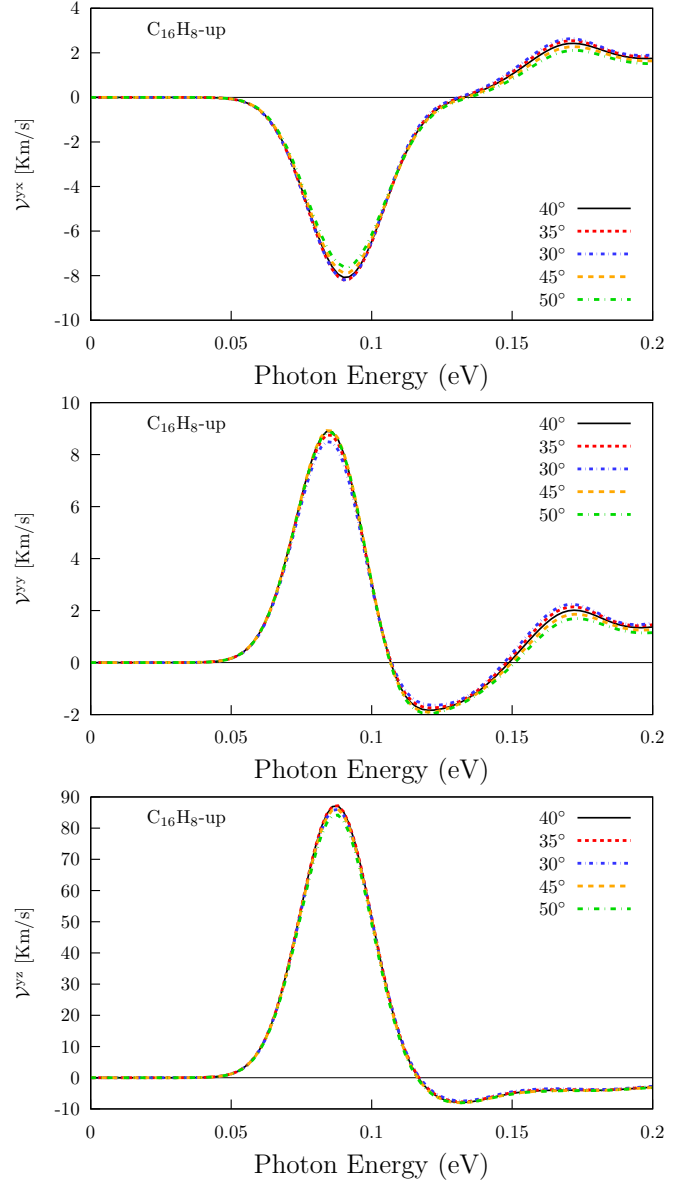


Figure 16: Cheking angle of incidence for  $yb$  components.



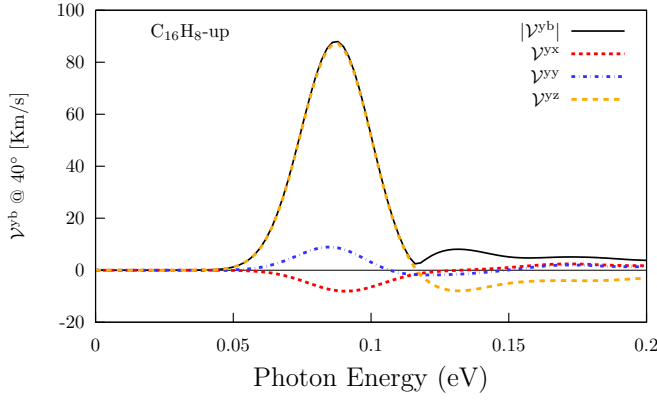


Figure 17: Three components of  $\gamma^y$  @  $40^\circ$ .

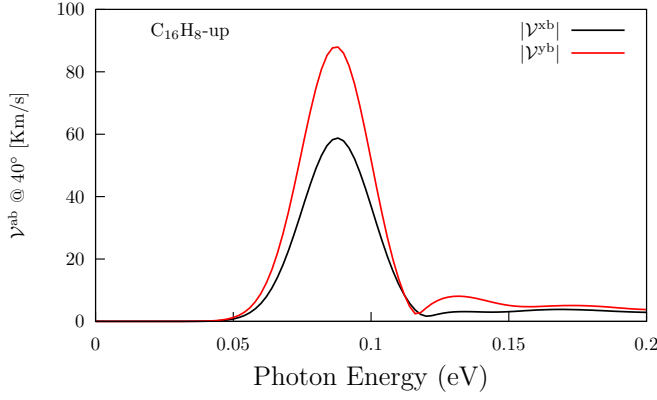


Figure 18: Comparisson of  $|\gamma^x|$  and  $|\gamma^y|$

### 3.2.3 $\gamma^x$ energy range 1.8–2.1 eV

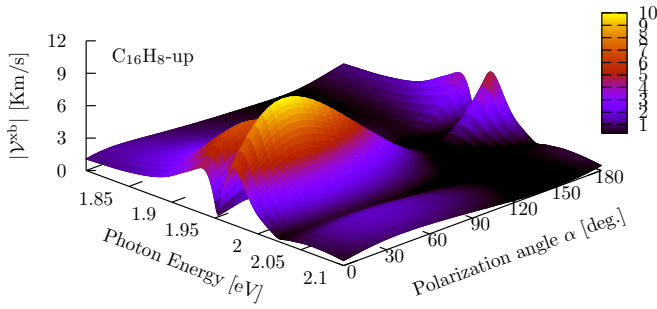


Figure 19: The most intense response for  $\gamma^x$  is for  $40^\circ$ .

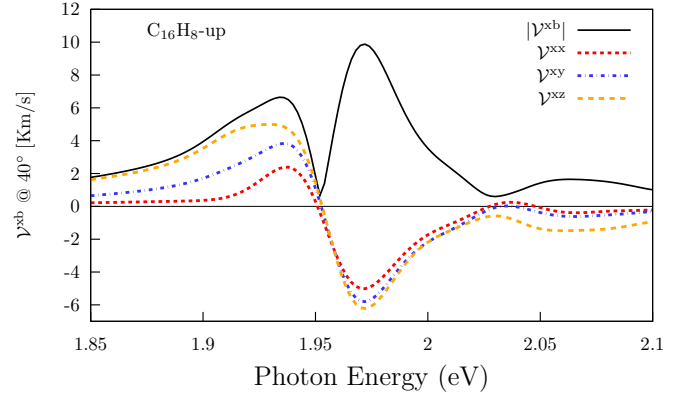


Figure 20: Three components of  $\gamma^x$  @  $40^\circ$ .

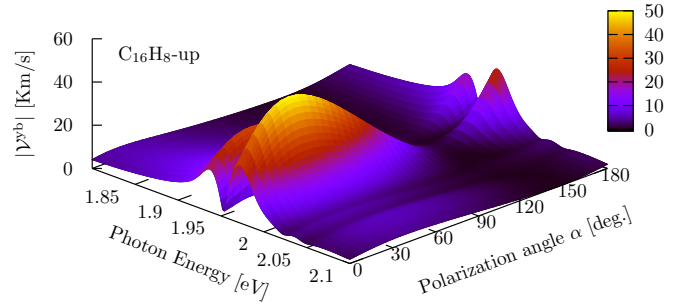


Figure 21: The most intense response for  $\gamma^y$  is for  $40^\circ$ .

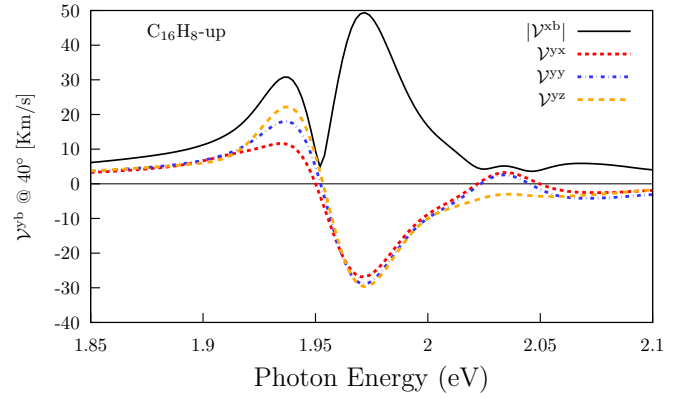


Figure 22: Three components of  $\gamma^y$  @  $40^\circ$ .

**3.2.4  $|\mathcal{V}^{ab}|$ , angles  $\theta$  and  $\varphi$ , layers, and comparison with CdSe and GaAs for the energy range of 0.0–0.2 eV.**

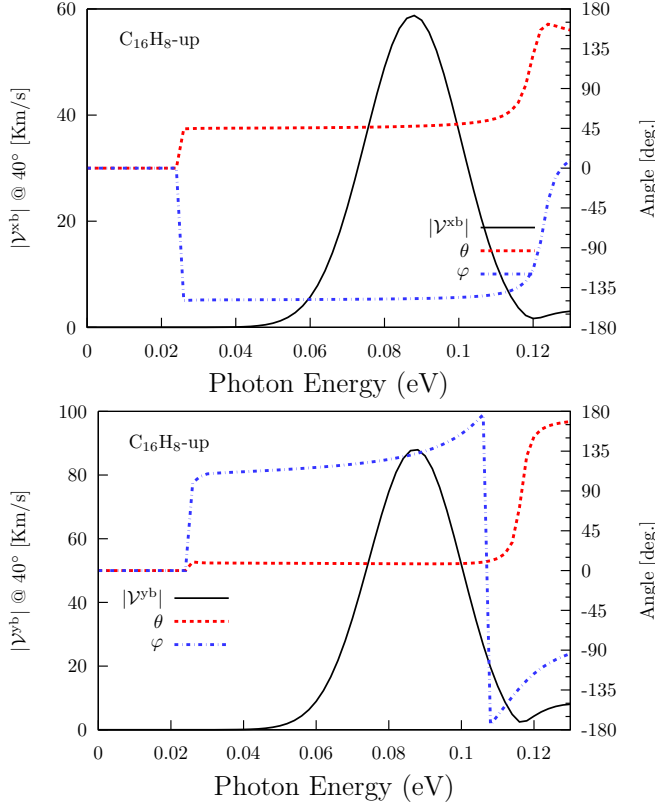


Figure 23:  $|\mathcal{V}^{ab}|$  (solid line, leftside scale) and the corresponding angles  $\theta$  and  $\varphi$  (dashed lines, rightside scale).

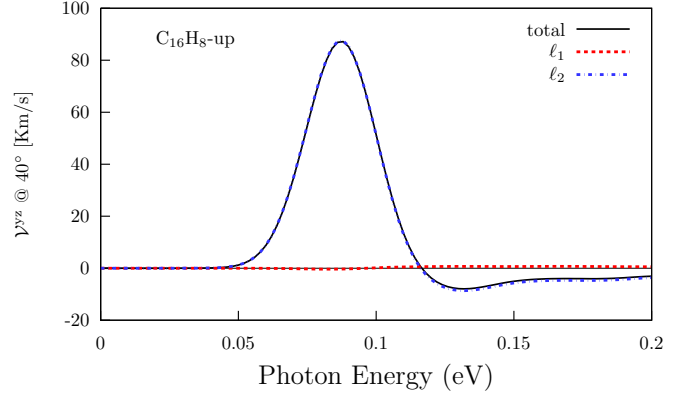


Figure 24: Layer decomposition for the most intense response:  $\mathcal{V}^{yz}$ .

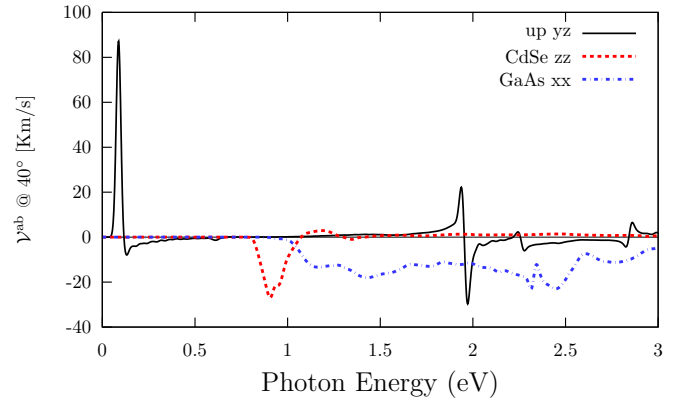


Figure 25: Comparisson of the most intense response vs the most intense responses of CdSe and GaAs.

**3.2.5  $|\mathcal{V}^{ab}|$ , angles  $\theta$  and  $\varphi$ , layers, and comparison with CdSe and GaAs for the energy range of 1.8–2.1 eV**

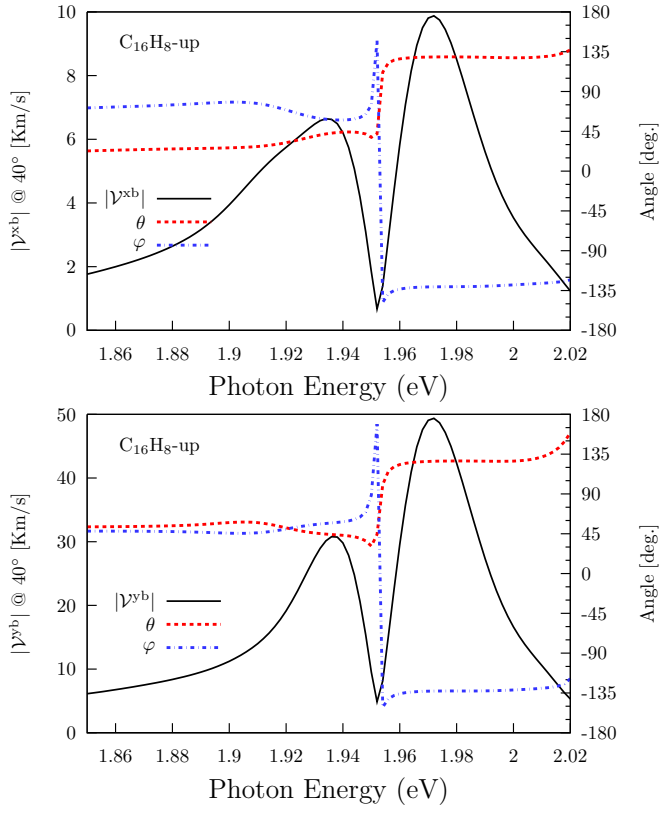


Figure 26:  $|V^{ab}|$  (solid line, leftside scale) and the corresponding angles  $\theta$  and  $\varphi$  (dashed lines, rightside scale).

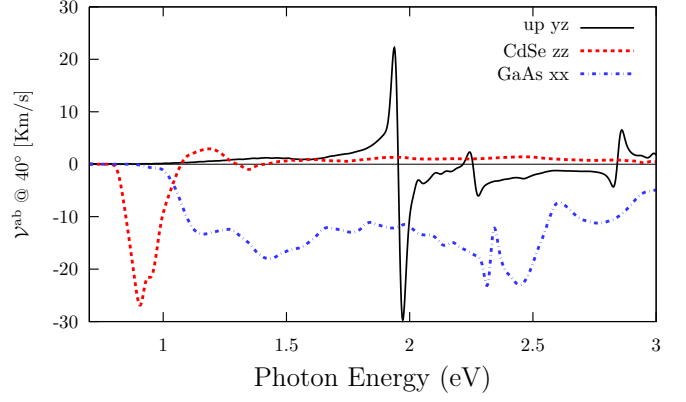


Figure 28: Comparisson of the most intense response vs the most intense responses of CdSe and GaAs.

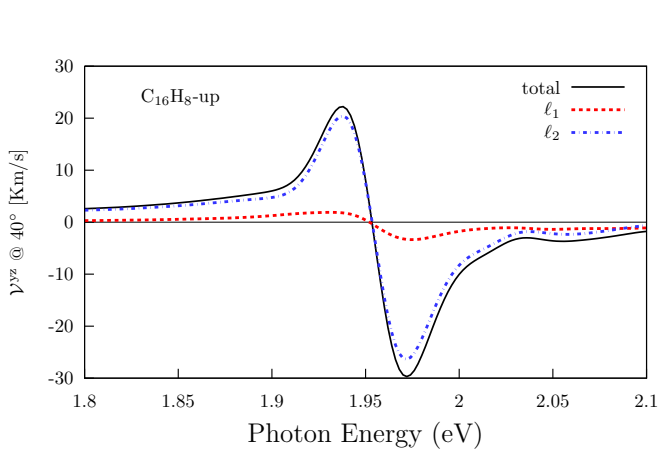
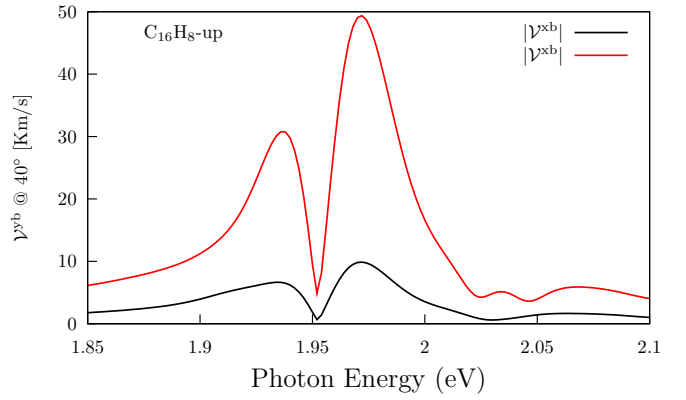


Figure 27: Layer decomposition for the most intense response:  $V^{yz}$ .



## References

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