

Reinaldo Arturo Zapata Peña presents

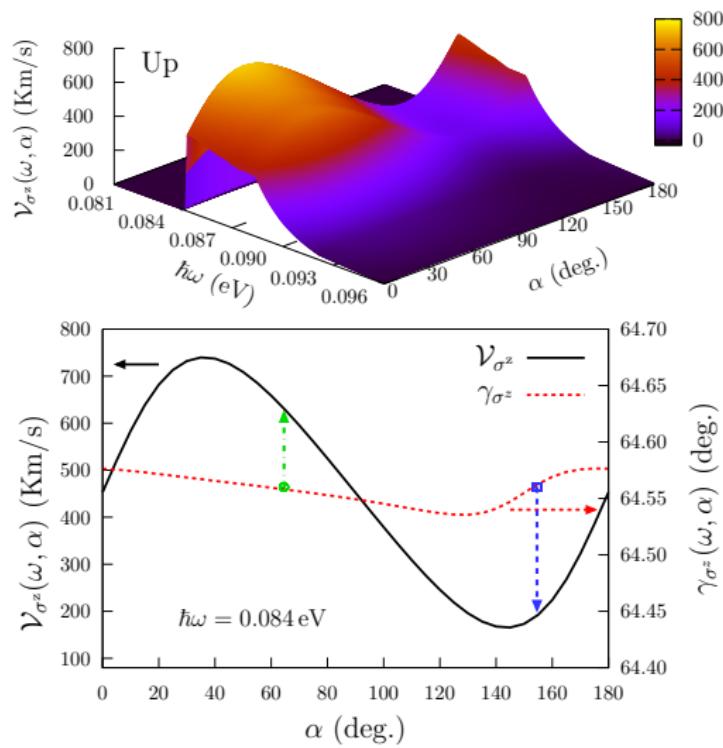
Novel Optical Effects in Functionalized Graphene: Formalism and Simulations

to earn the degree of Doctor of Science (Optics)



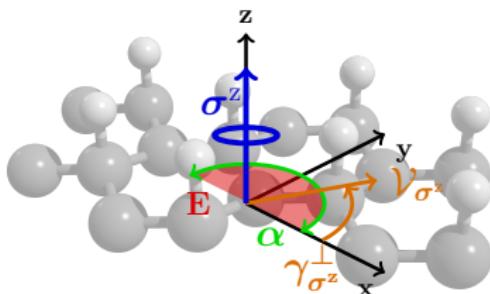
CENTRO DE INVESTIGACIONES
EN ÓPTICA, A.C.

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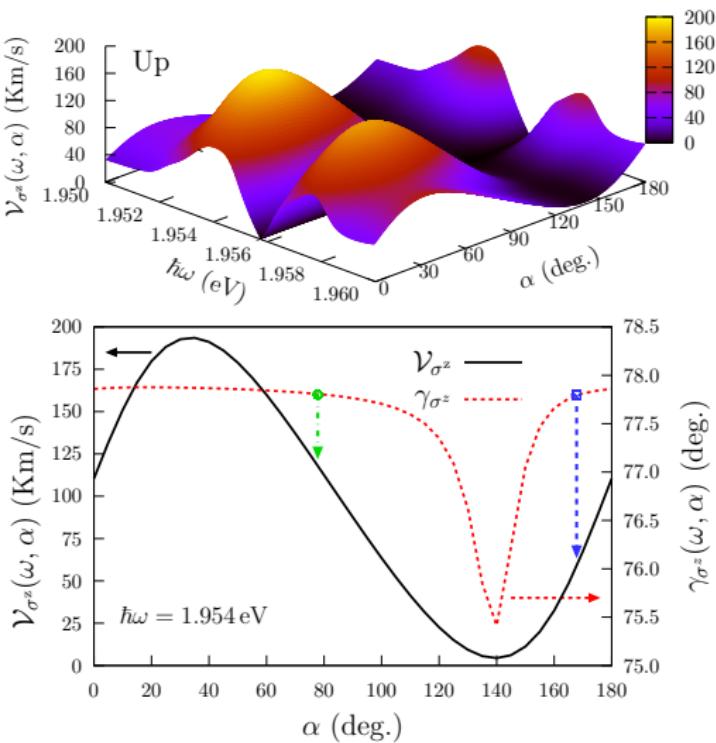
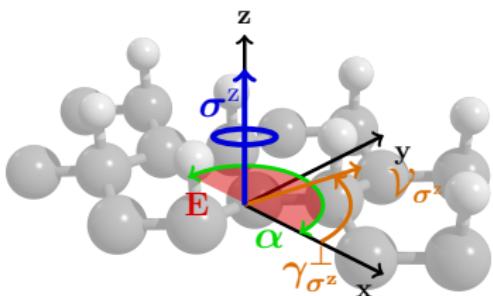


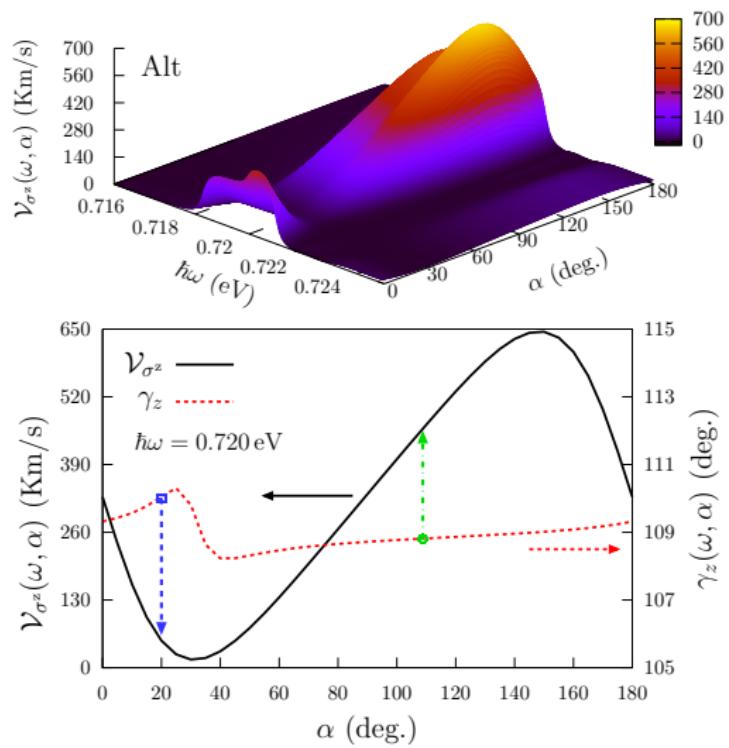
For *up*, when the spin is polarized along z the spin velocity V_{σ^z} :

- Is maximized for $\hbar\omega = 0.084$ eV
- The absolute maxima is 739.7 Km/s for $\alpha = 35^\circ$
- The velocity is directed almost at a constant angle $\gamma_{\sigma^z} = 64.5^\circ$



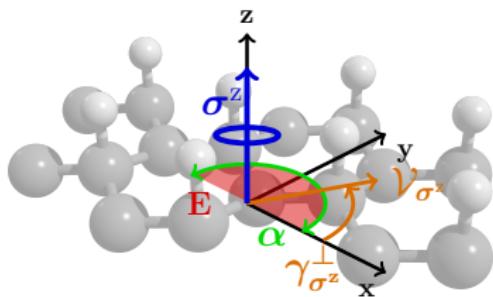
- A local maxima is found for $\hbar\omega = 1.954 \text{ eV}$ (634 nm, visible red)
- The maxima is 193.5 Km/s for $\alpha = 35^\circ$
- The velocity angle γ_{σ^z} has values between 75.5° and 77.8°

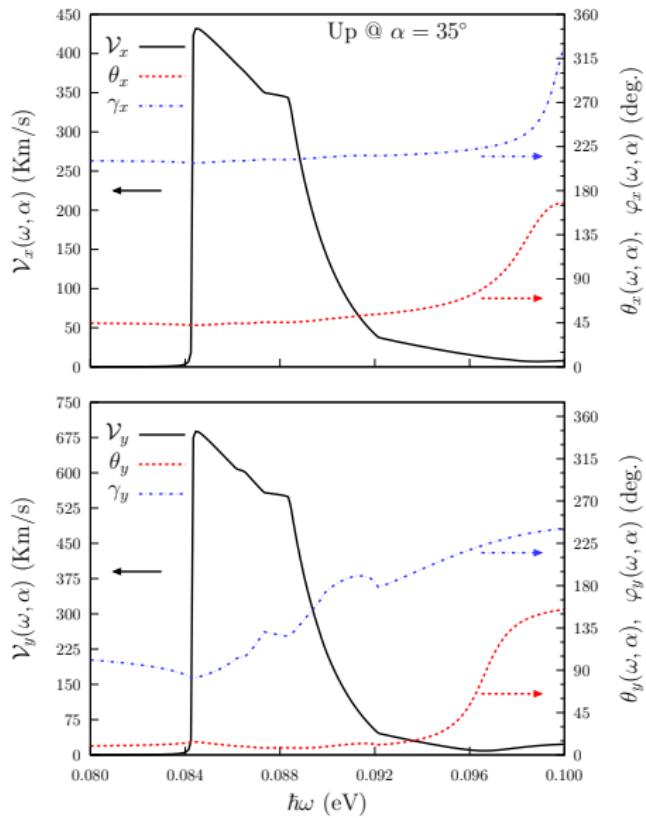


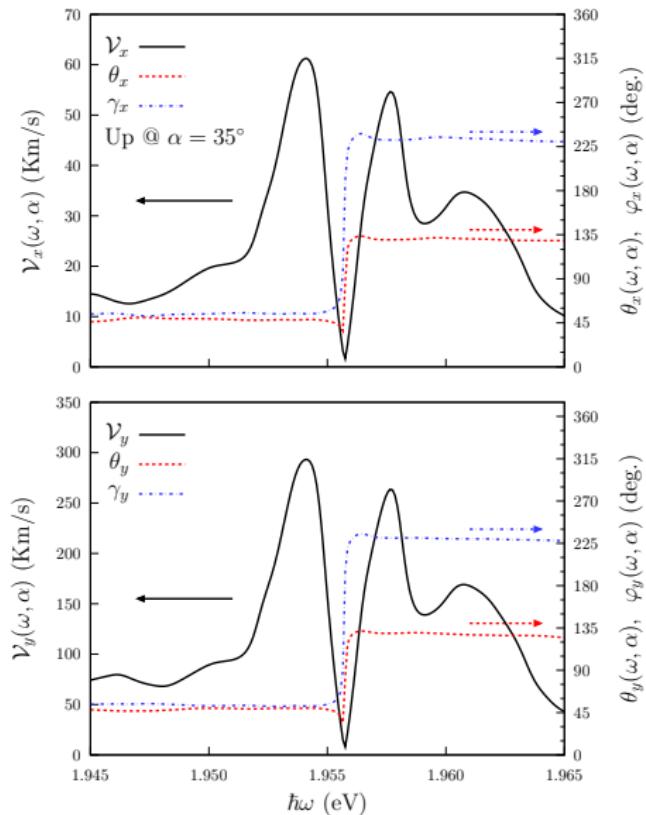


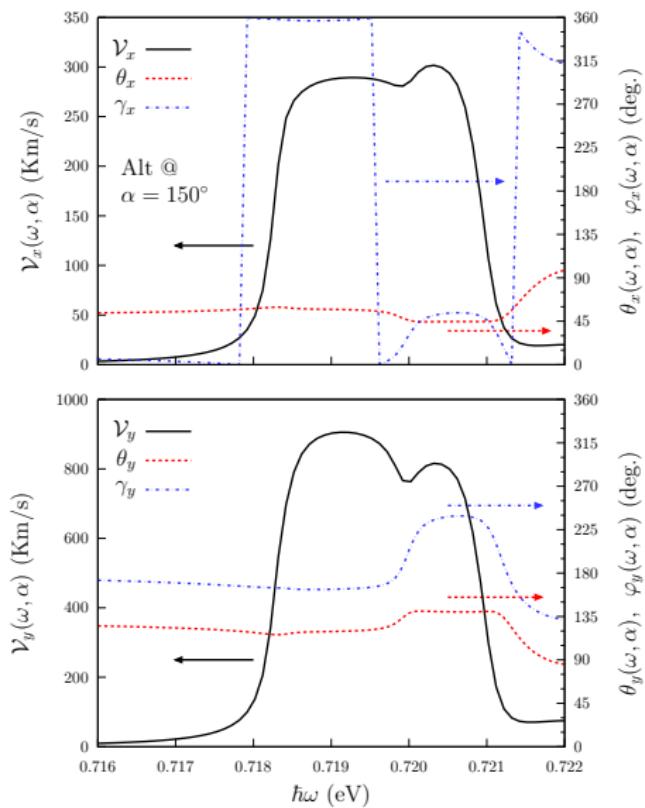
For *alt*, when the spin is polarized along z the spin velocity V_{σ^z} :

- Is maximized for $\hbar\omega = 0.720$ eV
- The absolute maxima is 644.9 Km/s for $\alpha = 150^\circ$
- The velocity is directed almost at a constant angle $\gamma_{\sigma^z} = 109^\circ$









Conclusions

- We found that the *up* is more spin-polarizable than the *alt.*
- The *up* structure is can achieve a larger injection current being the response bigger than other structures but being overcome by the CdSe.
- Both structures are excellent candidates to generate second harmonic, particularly the *up* one.
- It is possible to generate pure-spin currents in our structures; also it is possible to control the spin orientation or the current direction making variations in the angle of the polarization of the incoming beam.