Nonlinear Optical Responses in Hydrogenated Graphene Structures

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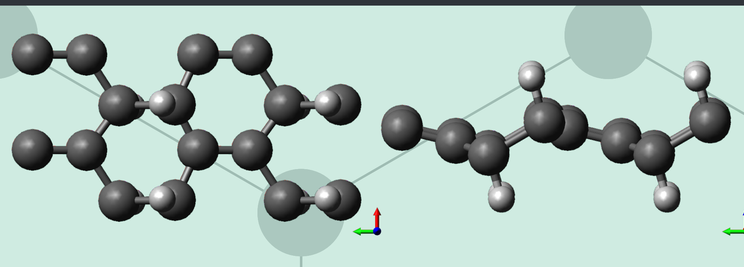
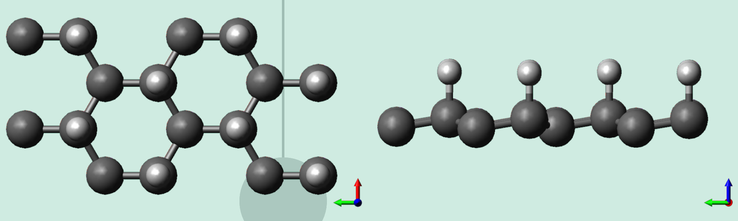
Introduction

Graphene has become a matter of interest in science and technology. The band-gap opening can be reached trough hydrogenation. We characterised the degree of spin polarization, optical current injection, and second harmonic generation in two hydrogenated graphene structures presenting a gap: $C_{16}H_8$-alt and $C_{16}H_8$-up. Our results show an anisotropic behaviour in the optical responses.

Structures

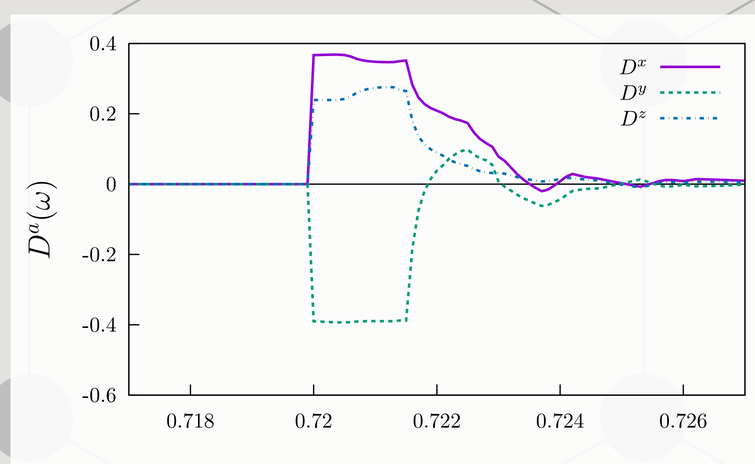


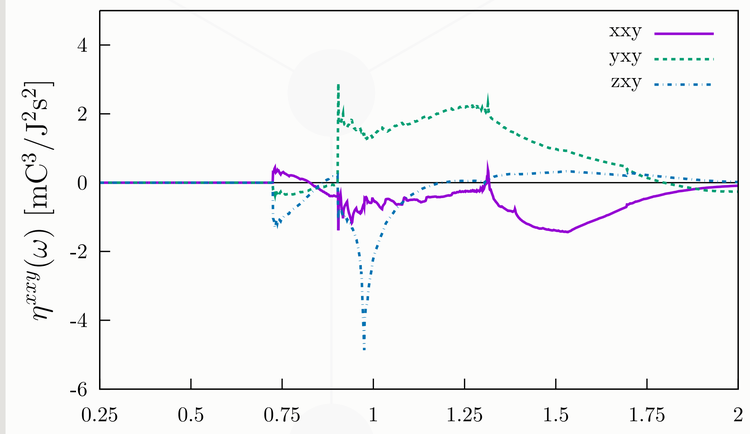
$C_{16}H_8$-alt, 50% hydrogenation

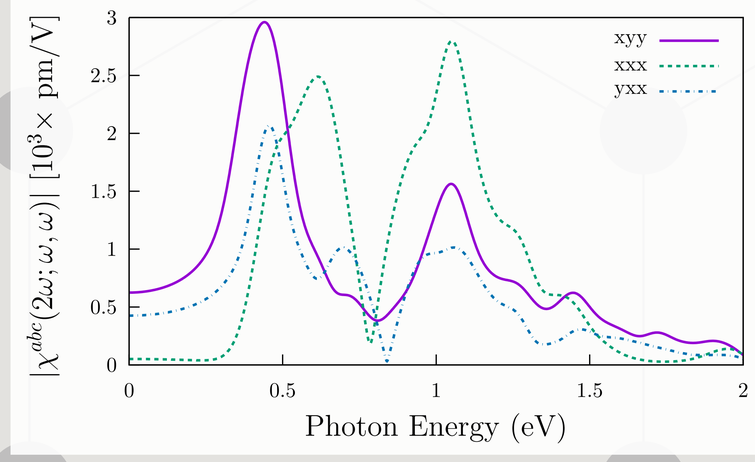


$C_{16}H_8$-up, 50% hydrogenation

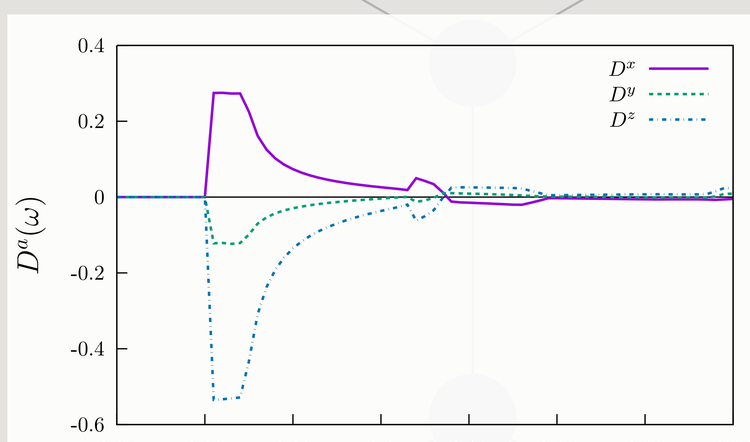
Results

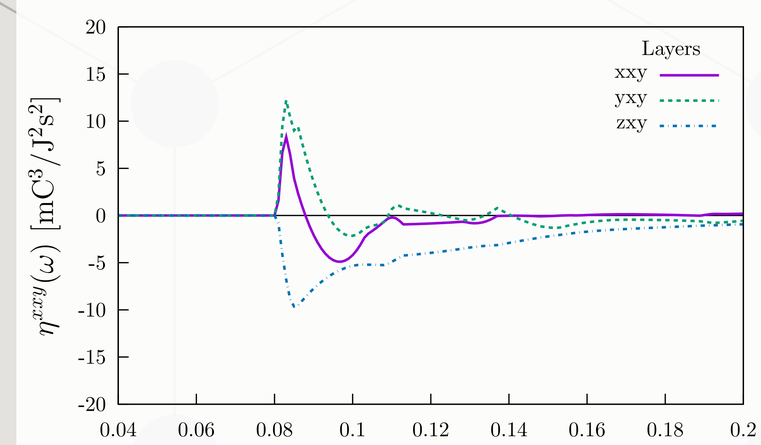


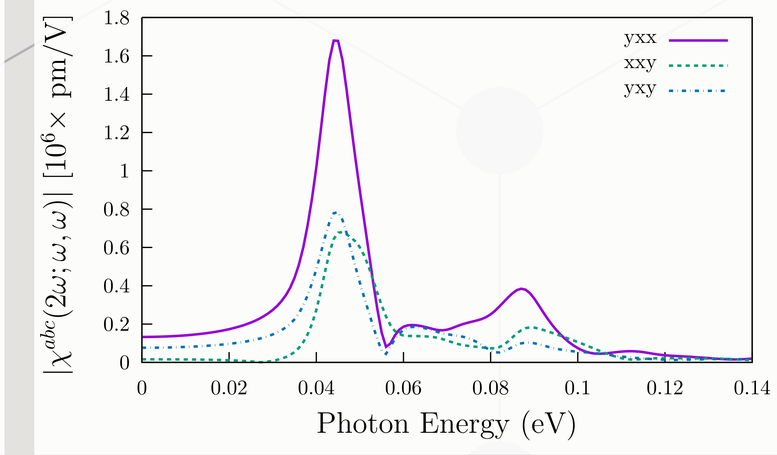




$C_{16}H_8$-alt responses







$C_{16}H_8$-up responses

Theory

Degree of spin polarization [1]:

$$\mathcal{D}^a(\omega) = \frac{2\zeta^{\mathrm{abc}}}{\hbar\left(\xi^{\mathrm{bb}}\xi^{\mathrm{cc}}\right)/2}$$

$$\zeta^{\mathrm{abc}}(\omega) = \frac{i\pi e^2}{\hbar^2}\int\frac{d^3k}{8\pi^3}\sum_{vcc'}{}'\mathrm{Im}\left[S^{\mathrm{a}}_{c'c}(\mathbf{k})r^{\mathrm{b}}_{vc'}(\mathbf{k})r^{\mathrm{c}}_{cv}(\mathbf{k}) + S^{\mathrm{a}}_{cc'}(\mathbf{k})r^{\mathrm{b}}_{vc}(\mathbf{k})r^{\mathrm{c}}_{c'v}(\mathbf{k})\right]\delta(\omega_{cv}(\mathbf{k})-\omega)$$

$$\xi^{\mathrm{ab}}(\omega) = \frac{2\pi e^2}{\hbar^2}\int\frac{d^3k}{8\pi^3}\sum_{vc} r^{\mathrm{a}}_{vc}(\mathbf{k})r^{\mathrm{b}}_{cv}(\mathbf{k})\delta(\omega_{cv}(\mathbf{k})-\omega)$$

Optical current injection tensor [2]:

$$\eta^{\mathrm{abc}}(0;\omega,-\omega) = \frac{i\pi e^3}{\hbar}\int\frac{d^3k}{8\pi^3}\sum_{vc}\Delta^{\mathrm{a}}_{cv}(\mathbf{k})\,\mathrm{Im}\left[r^{\mathrm{b}}_{cv}(\mathbf{k})r^{\mathrm{b}}_{vc}(\mathbf{k})\right]\delta(\omega_{cv}(\mathbf{k})-\omega)$$

Second harmonic generation tensors [3]:

$$\mathrm{Im}[\chi^{\mathrm{abc}}_{e,\omega}] = \int\frac{dk^3}{8\pi^3}\sum_{vc}\sum_{q\neq(v,c)}\frac{1}{\omega^{\Sigma}_{cv}}\left[\frac{\mathrm{Im}[\mathcal{V}^{\Sigma,\mathrm{a}}_{qc}\{r^{\mathrm{b}}_{cv}r^{\mathrm{c}}_{vq}\}]}{(2\omega^{\Sigma}_{cv}-\omega^{\Sigma}_{cq})} - \frac{\mathrm{Im}[\mathcal{V}^{\Sigma,\mathrm{a}}_{vq}\{r^{\mathrm{c}}_{qc}r^{\mathrm{b}}_{cv}\}]}{(2\omega^{\Sigma}_{cv}-\omega^{\Sigma}_{qv})}\right]\delta(\omega^{\Sigma}_{cv}-\omega)$$

$$\mathrm{Im}[\chi^{\mathrm{abc}}_{e,2\omega}] = \int\frac{dk^3}{8\pi^3}\sum_{vc}\frac{4}{\omega^{\Sigma}_{cv}}\left[\sum_{v'\neq v}\frac{\mathrm{Im}[\mathcal{V}^{\Sigma,\mathrm{a}}_{vc}\{r^{\mathrm{b}}_{cv'}r^{\mathrm{c}}_{v'v}\}]}{2\omega^{\Sigma}_{cv'}-\omega^{\Sigma}_{cv}} - \sum_{c'\neq c}\frac{\mathrm{Im}[\mathcal{V}^{\Sigma,\mathrm{a}}_{vc}\{r^{\mathrm{c}}_{cc'}r^{\mathrm{b}}_{c'v}\}]}{2\omega^{\Sigma}_{c'v}-\omega^{\Sigma}_{cv}}\right]\delta(\omega^{\Sigma}_{cv}-2\omega)$$

Conclusions

We obtained maximum percentages of the degree of spin polarization of 48% and 68% for the alt and up structures, respectively. It is also possible to optically generate injection current and second harmonic in the alt and up structures.

Information

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[1] PRB 85, 165324 (2012)
[2] PRB 84, 195326 (2011)
[3] PRB 91, 075302 (2015)

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