

Nonlinear Optical Responses in Hydrogenated Graphene Structures

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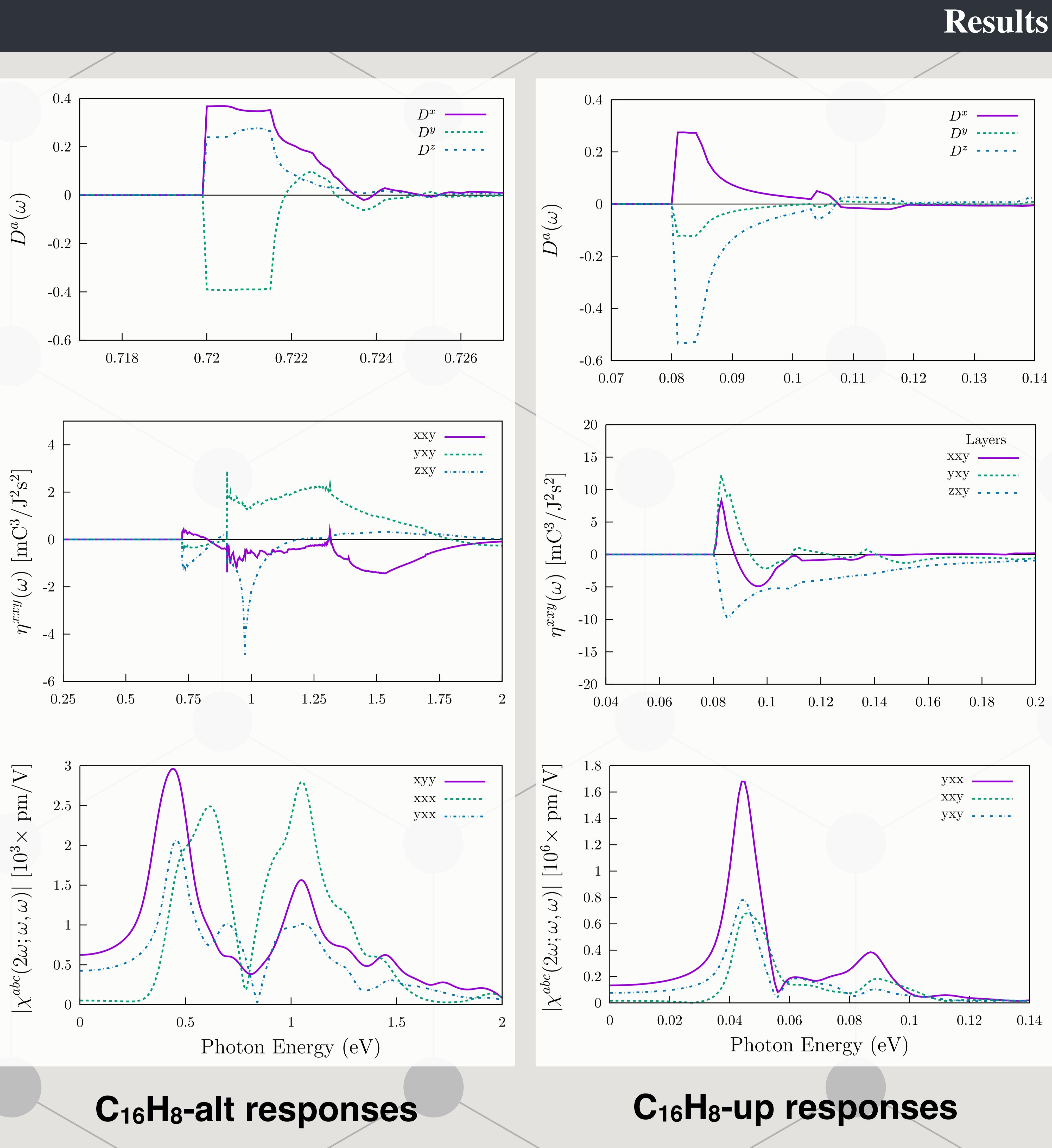
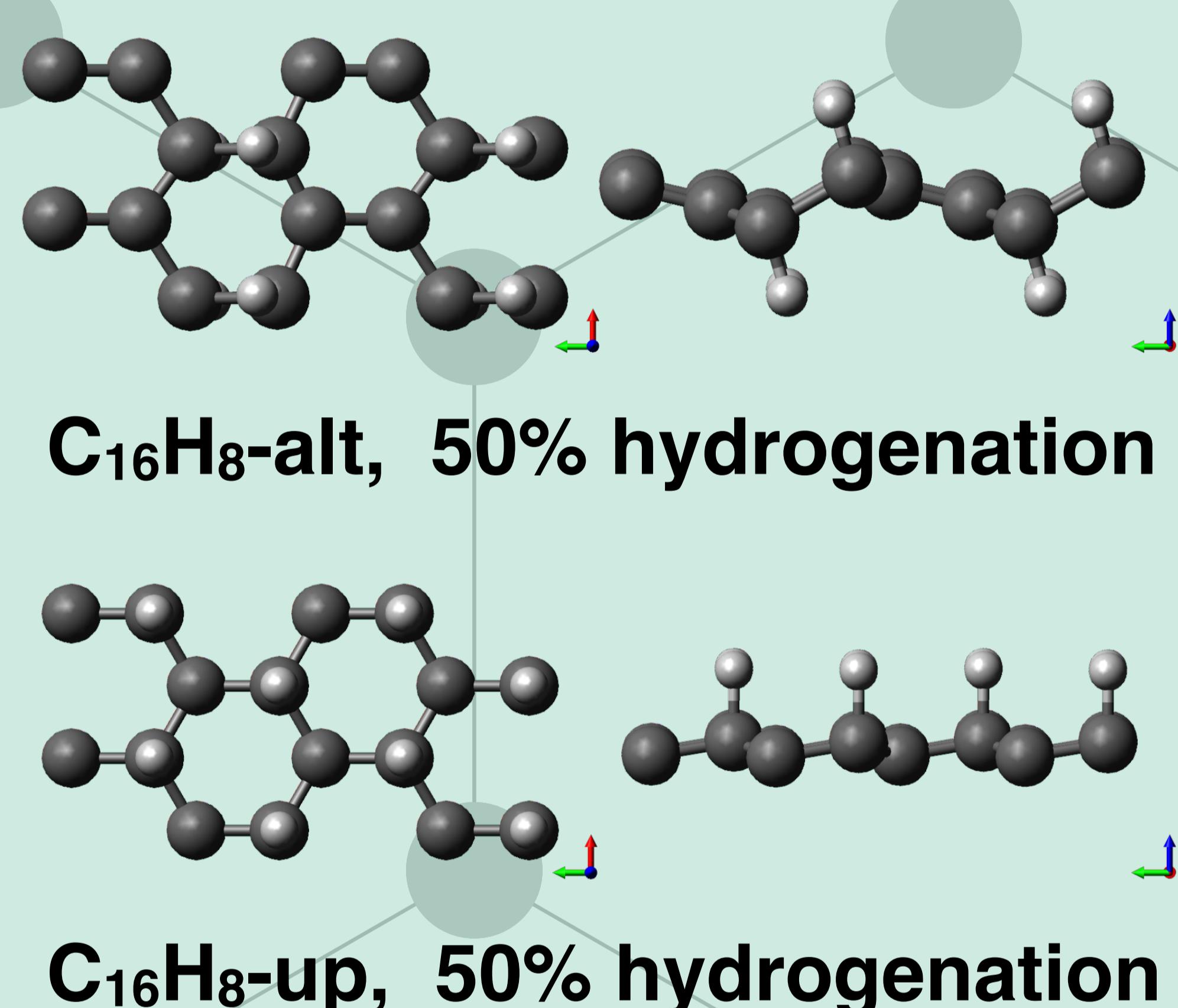
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Introduction

Graphene has become a matter of interest in science and technology. The band-gap opening can be reached through hydrogenation. We characterised the degree of spin polarization, optical current injection, and second harmonic generation in two hydrogenated graphene structures presenting a gap: C₁₆H₈-alt and C₁₆H₈-up. Our results show an anisotropic behaviour in the optical responses.

Structures



Results

Degree of spin polarization [1]:

$$\begin{aligned} D^a(\omega) &= \frac{2\zeta^{abc}}{\hbar(\xi^{bb}\xi^{cc})/2} \\ \zeta^{abc}(\omega) &= \frac{i\pi e^2}{\hbar^2} \int \frac{d^3k}{8\pi^3} \sum_{vc'}' \text{Im} [S_{c'c}^a(\mathbf{k}) r_{vc'}^b(\mathbf{k}) r_{cv}^c(\mathbf{k}) + S_{cc'}^a(\mathbf{k}) r_{vc}^b(\mathbf{k}) r_{c'v}^c(\mathbf{k})] \delta(\omega_{cv}(\mathbf{k}) - \omega) \\ \xi^{ab}(\omega) &= \frac{2\pi e^2}{\hbar^2} \int \frac{d^3k}{8\pi^3} \sum_{vc} r_{vc}^a(\mathbf{k}) r_{cv}^b(\mathbf{k}) \delta(\omega_{cv}(\mathbf{k}) - \omega) \end{aligned}$$

Optical current injection tensor [2]:

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

Second harmonic generation tensors [3]:

$$\begin{aligned} \text{Im}[\chi_{e,\omega}^{abc}] &= \int \frac{dk^3}{8\pi^3} \sum_{vc} \sum_{q \neq (v,c)} \frac{1}{\omega_{cv}^\Sigma} \left[\frac{\text{Im}[\mathcal{V}_{qc}^{\Sigma,a} \{r_{cv}^b r_{vq}^c\}]}{(2\omega_{cv}^\Sigma - \omega_{cq}^\Sigma)} - \frac{\text{Im}[\mathcal{V}_{vq}^{\Sigma,a} \{r_{qc}^c r_{cv}^b\}]}{(2\omega_{cv}^\Sigma - \omega_{qv}^\Sigma)} \right] \delta(\omega_{cv}^\Sigma - \omega) \\ \text{Im}[\chi_{e,2\omega}^{abc}] &= \int \frac{dk^3}{8\pi^3} \sum_{vc} \frac{4}{\omega_{cv}^\Sigma} \left[\sum_{v' \neq v} \frac{\text{Im}[\mathcal{V}_{vc}^{\Sigma,a} \{r_{cv'}^b r_{v'v}^c\}]}{2\omega_{cv'}^\Sigma - \omega_{cv}^\Sigma} - \sum_{c' \neq c} \frac{\text{Im}[\mathcal{V}_{vc}^{\Sigma,a} \{r_{cc'}^c r_{c'v}^b\}]}{2\omega_{c'v}^\Sigma - \omega_{cv}^\Sigma} \right] \delta(\omega_{cv}^\Sigma - 2\omega) \end{aligned}$$

Theory

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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