Nonlinear optical responses in hydrogenated graphene structures

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Abstract.

Abstractauthoren We present a theoretical study of the optical spin injection, optical current injection, and second harmonic generation of two 50% hydrogenated graphene structures: Cinline imageHinline image-alt and Cinline imageHinline image-up. Optical spin injection, under the incidence of circularly polarized light onto nonmagnetic semiconductors, creates spin-polarized electrons in the conduction bands. Optical current injection and second-harmonic generation are nonlinear second-order effects that are allowed in materials without inversion symmetry. The results are calculated in a full electronic band structure scheme within DFT in the LDA approximation. Our results show an anisotropic behavior in the optical responses of the spin, the current injection, and second harmonic generation. We obtained maximum absolute magnitudes of the degree of spin polarization of 61 and 64% for the alt and up structures, respectively, and it is also possible to optically generate an injection current coming mainly from the carbon layer on both alt and up systems. Besides, we found that both structures are excellent candidates for second harmonic generation.