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Anisotropic excitonic effects on 2D black phosphorus: an ab initio approach considering the DFT-1/2 method

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Abstract

Among the two-dimensional (2D) materials, phosphorene, obtained from Black Phosphorus (BP) has gained great interest. Along with its unique electronic properties, phosphorus is one of the most prominent examples of anisotropic materials, as it has an anisotropic band structure, considering only in-plane coordinates. This anisotropy is often reflected in the optical properties of the material, resulting in plasmonic states with different frequencies to polarize light in different directions and thus, the scattering of a polariton plasmon becomes hyperbolic. In-plane hyperbolic polaritons, natural in layered materials, have been demonstrated in MoO3 and Wte2, which are based on phonon and plasmon resonances, respectively. In recent works, it was predicted that the BP monolayer naturally hosts hyperbolic exciton-polaritons, which opened a new perspective of natural hyperbolic polaritons in the plane, based on excitons rather than phonons or plasmons [1]. From the theoretical point of view the study of a procedure to compute optical spectra including excitonic effects and approximated quasiparticle corrections with reduced computational effort is of great importance and could open an avenue for the study of hyperbolic exciton-polaritons, considering not only monolayer, but also few layers of anisotropic materials.

In this work, we investigated the electronic and optical properties of monolayer and bilayer of black phosphorus (BP). The excitonic effects on optical spectra are included by solving the Bethe–Salpeter equation, considering quasiparticle eigenenergies and respective wavefunctions obtained within DFT-1/2 method [2]. Surprisingly, despite both valence and conduction bands having the same orbital character in BP, the DFT-½ method proved to be effective in obtaining reasonable band gaps, comparable to other theoretical methods as HSE and GW, as well as, to the experimental data. The anisotropic dielectric function (real and imaginary parts), initially made with and without the contribution of excitonic effects, was obtained and compared with the available data. From initial analysis, evidence of the existence of hyperbolic exciton-polaritons was observed. The results showed that the DFT-½ method can provide an insight on the electronic and optical properties of these materials.

References

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