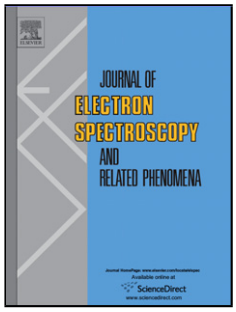


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# Excitonic effects in the K and $L_{2,3}$ edges spectra of bulk and monolayer black phosphorus from first-principles

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## *Highlights*

- Both bulk and monolayer black phosphorus show strong anisotropy in their core absorption spectra.
- The electron-hole coupling and formation of the bound exciton have a significant effect on the edge spectra of both bulk and monolayer BP in a way that the excitonic effects intensely modify the oscillator strengths and the energy positions of the main spectral structures.
- Moving from bulk to monolayer, all the K and $L_{2,3}$ absorption spectra are red-shifted.
- Considering the excitonic effects leads to the red-shift of the core spectra.
- Decomposition of $L_{2,3}$ edge to $L_2$ and $L_3$ edges indicates that the contribution of the $L_3$ edge is dominant.
- Local densities of states calculations show that *p*-like and *d*-like states of phosphorus atoms play the main role in the electron transitions of K and $L_{2,3}$ edges spectra, respectively.

## Abstract

*In this study, the K and $L_{2,3}$ X-ray absorption near edge structure (XANES) of bulk and monolayer black phosphorus (BP) were calculated and compared. Calculations were performed in two different levels of theory, with and without considering the excitonic effects. The present calculations indicated that both bulk and monolayer BP showed strong anisotropy in their core absorption spectra. The results demonstrated that the electron-hole coupling and formation of*