عنوان مقاله:

First-principles calculations on photocatalytic activity of ZnWO4 doped with Lithium

محل انتشار:

سومین کنفرانس علوم و فناوری های شیمی کاربردی: شیمی زمین و شیمی محیط زیست (سال: 1399)

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خلاصه مقاله:

In this paper, ZnWO4 -doped with of Li. dielectric and the consequent optical refraction constants have been calculated according to density function theory (DFT) and by using CASTEP calculation method. GGA approximation has been used for correlation and exchange effects and results have been compared by experimental results. The calculations showed that doped ZnWO4 with Li (18.8%), dielectric constant will increase and structure of the main spectrum goes toward less energy which satisfies the corresponding experimental data result. The theoretical data reveal that main contributors in the valence band of ZnWO4 are the Zn 3d-, W 5d- and O 2p-like states: the Zn 3d- and W 5d-like states contribute mainly at the bottom, whilst the O 2p-like states at the top of the valence band, with also significant portions of contributions of the above states throughout the whole valence-band region of the tungstate under study. The DFT calculations suggest that the Li doping and the induced OVs can narrow the band gap which enhances photocatalytic activity in the visible light region.

کلمات کلیدی:

(hotocatalytic activity, Castep, Dielectric constant, Optical properties, Zinc tungstate (ZnWO4