

Abstract Submitted
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Effect of Nitrogen Doping on the Electronic and Optical Properties of TaON NABIL AL-AQTASH, FLORIN APOSTOL, RENAT SABIRIANOV, University of Nebraska at Omaha — TaON is considered as a potential candidate as a visible-light responsive photocatalyst. We report the results of ab initio studies of electronic structure of TaON in monoclinic and hypothetical cubic phases using VASP code. Specifically, we show that the position of conduction and valence band can be modified by varying the nitrogen (N) concentration in $\text{TaO}_{1+x}\text{N}_{1-x}$. The bandgap decreases monotonically with the increase of N concentration from near 2.7eV to just over 1.1eV (i.e. by 230%) when N concentration is reduced from $x=0.5$ to 1.5. The bandgap reduction is mostly associated with the change in the position of the valence band, while the conduction band is not sensitive to nitrogen content. We calculated the optical absorption spectra and discuss the effect of nitrogen doping on the photocatalytic activity of oxinitrides.

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