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# Doping Induced Structural Transformation in Tungsten

## Trioxide

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### ABSTRACT

Effects of dopants on structural stability of monoclinic  $\text{WO}_3$  were studied using density functional theory. Transformation from monoclinic to cubic crystal structures was obtained by gradually increasing doping concentrations of both rhenium (Re) and electrons inside the monoclinic  $\text{WO}_3$ , whereas a large distortion of  $\text{WO}_6$  octahedra was observed by gradually increasing doping concentrations of both niobium (Nb) and holes inside the monoclinic  $\text{WO}_3$ . It was verified that  $\text{Re}_x\text{W}_{1-x}\text{O}_3$  has a cubic structure if  $x$  is larger than 0.375, and the transformation from monoclinic to cubic structure is mainly dependent on the occupancy of the W  $5d$  orbital. The elastic characteristics of the  $\text{Re}_x\text{W}_{1-x}\text{O}_3$  decrease with the increase of the content of Re in the range of  $0.375 \leq x \leq 0.875$ .

Keywords: Tungsten Trioxide; Phase transformation; Doping; Density functional theory

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