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Phase Transformations upon Doping in Tungsten Trioxide[1] WENNIE WANG, Univ of California - Santa Barbara , ANDERSON JANOTTI[2], University of Delaware, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara — Tungsten trioxide (WO_3) is an emerging semiconductor material, with a growing number of applications in Li-ion batteries, photocatalysis, gas sensors and electrochromic devices. As an electrochromic material, WO_3 turns from transparent to blue upon doping with monovalent species. Due to it having an empty A-site in the ABO_3 perovskite structure, high doping concentrations are possible through intercalation. Tungsten trioxide has been experimentally shown to transform from the ground-state monoclinic symmetry to cubic symmetry with increasing monovalent doping [1]. We use first-principles calculations to understand this transformation. Our calculations show that the addition of electrons to the conduction band is a primary driver of the phase transformation. We quantify the energetics and structural aspects of this transformation using density functional theory, allowing us to elucidate the mechanism. Comparison with experiment, role of the dopant species, and implications of structural changes for device applications will be discussed. [1] Q. Zhong, J. Dahn, K. Colbow. *Phys. Rev. B* **46** 2554 (1992).

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