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Understanding the Oxygen Vacancy in Tungsten Trioxide WENNIE WANG, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Dept., Univ of California, Santa Barbara — Tungsten trioxide (WO_3) has a variety of applications in gas sensors, photocatalysis, and smart windows. As an electrochromic BO_3 perovskite, WO_3 turns from transparent to blue upon doping. This color change is correlated with a drop in transmittance of near-IR radiation, and is used in smart windows for energy efficiency. In addition to monovalent species doping that modulates optical properties, oxygen deficiencies have been found to have a similar electrochromic effect. The influence of oxygen vacancies on electronic structure and how it corresponds to electrochromic behavior remains a topic of debate. In this work, we examine the oxygen vacancy in monoclinic WO_3 and its influence on electronic structure using density functional theory with a hybrid functional. We investigate the relative stability of different charge states and its implications for electrical properties, such as conductivity and electrochromism. We find oxygen vacancies to be shallow donors, and explore similarities and differences with monovalent species doping. Finally, we compare our theoretical findings with experiment to elucidate how vacancies may contribute to electrochromic behavior. This work is supported by DOE and NSF.

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