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Electronic structure of oxygen di-vacancies on the (110) surface of rutile WILLIE MADDOX, BRANDEN KAPPES, CHRISTIAN CIOBANU, Department of Engineering, Colorado School of Mines — We report the results of electronic structure calculations for the reduced surface of rutile (110). We have performed density functional theory calculations in the framework Hubbard-corrected generalized gradient approximation (GGA+U) to investigate the electronic signatures of single and di-vacancies on rutile (110) slabs, both neutral and positively charged. We have also carried out Bader charge analysis to evaluate the charge transfer that occurs upon the reduction of the rutile surface. We observe n-type character for the neutral systems and p-type character for the positive slabs. For U=3 eV, we observe mid-gap states for the neutral system, while for U=6 eV, we observe mid-gap states for the positively charged system as well. Bader analysis shows that the atoms associated with mid-gap states are those that experience a larger charge transfer. The dependence of the band gap on the U parameter was also investigated, and the results were compared with experimental observations in the literature for both electronic properties and for structural atomic relaxations.

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