

Abstract Submitted  
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**First Principles Study of Formation Energies and Diffusion Mechanisms of Native Point Defects in Rutile  $\text{TiO}_{2-x}$**  HAKIM IDDIR, SERDAR OGUT, University of Illinois at Chicago, NIGEL BROWNING, University of California at Davis — We present results from first principles calculations for the formation energies and diffusion mechanisms of the oxygen vacancy ( $\text{V}_\text{O}$ ), titanium interstitial ( $\text{Ti}_\text{I}$ ) and titanium antisite ( $\text{Ti}_\text{O}$ ) point defects in reduced rutile  $\text{TiO}_{2-x}$ . The calculations are performed in large supercells containing 240 to 270 atoms using the *ab initio* pseudopotential total energy method. As expected, the formation energy of  $\text{Ti}_\text{O}$  is found to be significantly higher than  $\text{V}_\text{O}$  and  $\text{Ti}_\text{I}$ , which have competitive formation energies as a function of the sample stoichiometry. The dominant charge states of  $\text{V}_\text{O}$  and  $\text{Ti}_\text{I}$  are found to be (2+) and (4+), respectively, for a wide range of the electron chemical potential. The calculated diffusion barriers for  $\text{Ti}_\text{I}^{4+}$  are lower than those of  $\text{V}_\text{O}^{2+}$ , and do not present a significant anisotropy between the (100) open channels and the (110) direction. In fact, the barrier for the diffusion of  $\text{Ti}_\text{I}^{4+}$  along the (100) open channels has an unexpectedly 0.1 eV higher barrier than along (110). The reasons for this observation and the implications of the present results are discussed in relation to bulk-defect assisted surface phenomena in rutile  $\text{TiO}_2$ .

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