Abstract Submitted
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First-principles determination of the electronic structure of native point defects and impurities in rutile TiO_2[1] JUN HE, Argonne National Laboratory, SUSAN SINNOTT, University of Florida — Density-functional theory calculations are used to determine the electronic structures of native point defects (Ti interstitials and O vacancies) and dopants (Al and Nb) in rutile TiO_2. The calculated densities of states (DOS) show that in pristine and defective structures that contain charged Ti interstitials or O vacancies, the lower conduction bands of the defective structures are shifted up in energy relative to the perfect structure. This shift leads to a broader lower conduction band that more readily promotes the formation of shallow donor levels. This effect is more pronounced in the case of Ti interstitials. We also find that the charge state of the Ti interstitial influences the extent of orbital overlap. The case of Al dopants is much more complex since Al can either be a donor or an acceptor. In the case of Al and Nb substitutional defects, the calculated DOS is similar to the DOS of the pristine structure.

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