Self-interaction corrected electronic structure of Ti4O7, TiO2 and Ti2O3 XIAOLIANG ZHONG, Argonne National Laboratory, IVAN RUNGGER, Trinity College, PETER ZAPOL, OLLE HEINONEN, Argonne National Laboratory — Titanium oxides have a range of applications in, e.g., catalysis and resistive switching. There are many oxide structures with different ground states and electronic properties that have to be understood for potential applications to be possible. We have studied rutile TiO_2, Ti_2O_3, and Magnéli phase Ti_4O_7 using density functional theory with self-interaction corrections to account for electronic correlations, which are important in these structures. The ground state of the low temperature (LT) phase of Ti_4O_7 is found to be a new semiconducting state with antiferromagnetic coupling between two sublattices. Depending on the charge screening strength, different Ti-O phases are best described by applying different values of an empirical parameter α, which represents the magnitude of the applied self-interaction correction. We will show that Pauli paramagnetism of the metallic high-temperature Ti_4O_7 phase is predicted using $\alpha \approx 0$, that the band gaps of small-gap LT-Ti_4O_7 and Ti_2O_3 are captured by $\alpha \approx 0$, while the large band gap of TiO_2 is reproduced using $\alpha \approx 0.9$. Nevertheless, restricting α to the standard value of 0.5 for transition metal oxides is found to be a good compromise describing reasonably well the electronic structures of all these oxides. We gratefully acknowledge the computing resources provided on Blues, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory. Argonne National Laboratory's work was supported under U.S. Department of Energy contract DE-AC02-06CH11357.

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