## Abstract Submitted for the MAR15 Meeting of The American Physical Society

Negative U behavior of  $TiO_{2-x}$  Magnéli and Corundum phases<sup>1</sup> ANTONIO CLAUDIO PADILHA, Universidade Federal do ABC, Santo André, Brazil, ALEXANDRE ROCHA, Universidade Estadual Paulista, São Paulo, Brazil, HANNES RAEBIGER, Yokohama National University, Yokohama, Japan, GUS-TAVO DALPIAN, Universidade Federal do ABC, Santo André, Brazil — The isolated oxygen vacancy is known to be a negative U defect in rutile TiO<sub>2</sub>. This effect manifests itself by a double donor level close to the conduction band. As oxygen is further removed,  $TiO_2$  no longer remains in the rutile structure and the Magnéli phases  $Ti_n O_{2n-1}$  ( $4 \le n \le 37$ ) are obtained. Those structures are characterized by ordered planes of oxygen vacancies (so-called shear planes) between rutile-like layers. Further removal of oxygen leads to the formation of  $Ti_3O_5$  and the corundum phase  $Ti_2O_3$ . In this work, we calculated using DFT+U the formation energy of several of these systems and show that these systems also have a double donor transition per oxygen vacancy. This means that these compounds as such also have negative Ubehavior, even though the vacancies are not isolated and the donor level is a broad delocalized impurity band close to the bottom of the conduction band. The relaxation energy for the doubly ionized system is larger than that of the singly ionized one, rendering the latter unstable.

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