Abstract Submitted
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Charge storage in oxygen deficient phases of TiO2: defect Physics without defects[1] A. C. M. PADILHA, Univ. Federal do ABC, Santo Andre, SP, Brazil, H. RAEBIGER, Yokohama Natl Univ., Yokohama, Japan, A. R. ROCHA, Univ. Est. Paulista, S SP, Brazil, G. M. DALPIAN, Univ. Federal do ABC, Santo Andre, Brazil — Defects in semiconductors can exhibit multiple charge states, which can be used for charge storage applications. Here we consider such charge storage in a series of oxygen deficient phases of TiO_2, known as Magnli phases. These Ti_nO_{2n-1} Magnli phases present well-defined crystalline structures, i. e., their deviation from stoichiometry is accommodated by changes in space group as opposed to point defects. We show that these phases exhibit intermediate bands with the same electronic transitions akin to interstitial Ti defect levels in TiO_2-rutile. Thus, the Magnli phases behave as if they contained a very large pseudo-defect density: $\frac{1}{2}$ per formula unit Ti_nO_{2n-1}. Depending on the Fermi Energy the whole material will become charged. These crystals are natural charge storage materials with a storage capacity that rivals the best known supercapacitors.

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