

Abstract Submitted  
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**Crystalline phase-stability of tantalum pentoxide<sup>1</sup>** SANTIAGO WALTON, Instituto Técnico Metropolitano, ITM, Medellin, Colombia, ANTONIO CLAUDIO PADILHA, GUSTAVO DALPIAN, Universidade Federal do ABC, UFABC, Santo André, Brazil, JORGE GUILLÉN, Universidad de Antioquia, Medellin, Colombia, DALPIAN'S RESEARCH GROUP COLLABORATION, GRUPO DE ESTADO SOLIDO COLLABORATION, GRITAD COLLABORATION — Memristive devices are attractive candidates to provide a paradigm change in memory devices fabrication. These new devices would be faster, denser and less power consuming than those available today. However, the mechanism of memristance is not yet well understood. It is believed that a voltage/current-driven phase transition occurs in the material, which leads to significant changes in the device's conductivity. In the particular case of tantalum-oxide-based devices the relevant crystalline phases are still a matter of debate. Some of these phases are not even completely known and there is no agreement about which model best explains the crystallographic results. In this work we have performed ab-initio DFT based calculations to study the structural properties of different phases (and models) of  $\text{Ta}_2\text{O}_5$  - the structure which is believed to exist inside Tantalum Oxide based devices. The equations of state for this material were constructed through first principles total energy calculations and we have also calculated the phonon frequencies at  $\Gamma$ . These results show that the most stable phase of this oxide (B- $\text{Ta}_2\text{O}_5$ ) is in fact composed of octahedral, instead of pentagonal (as L- $\text{Ta}_2\text{O}_5$ ) or hexagonal (as  $\delta$ - $\text{Ta}_2\text{O}_5$ ) bipyramids.

<sup>1</sup>Fapesp, CNPq, Capes, CODI-UdeA

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