# Resistive Switching in RRAM Devices through First Principles Calculation: Oxygen Vacancy-Induced Electron Conduction Path in $HfO_2$

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## INTRODUCTION

The electrically induced nanoscale resistive switching in resistance random access memory (RRAM) devices gains considerable attention as a promising non-volatile memory device [1]. From among the different structures of RRAM devices, the metal-insulator-metal sandwiched type structure mostly incorporates with it a transition metal oxide (TMO) insulator material that alters its resistive property upon subject to moderate amount of set and reset pulse voltage. This "ON-OFF" resistive switching has been exemplified in various experimental studies [1,2] but the basic mechanism at the atomic level is still unclear. Here, we employed first principles calculation based on density functional theory (DFT) to analyze the mechanism of resistive switching through a known TMO used in RRAM devices, $HfO_2$.

## RESISTIVE SWITCHING THROUGH OXYGEN VACANCIES

Experimental reports related to determining the switching mechanism in TMO-based RRAM [2] shows the existence of rowed (aligned) oxygen vacancies within the bulk TMO material upon subject to a relatively large amount of forming voltage. This causes change in the resistive property of the TMO from having insulator-like to having metallic-like properties. Thereafter, sufficiently small amount of set and reset pulse voltage is needed for the resistive switching. Therefore, the presence of rowed oxygen vacancies in $HfO_2$ was analyzed using DFT where results of the total density of states (TDOS) plots for bulk $HfO_2$ with rowed oxygen vacancies (Fig. 1) and plus charge carrier trapping (Fig.2) shows metallic properties [3]. This electron conduction path was also confirmed through the partial charge density distribution (Fig. 3) along the band crossing the Fermi level. Moreover, it was confirmed from the electrode(Ta)-TMO interaction that the layers of the TMO near the electrode interface have metallic properties with and without the presence of oxygen vacancies (Fig. 4). We thereby proposed a mechanism of resistive switching (Fig. 5) where oxygen vacancy migration from the interface layers to the bulk of the TMO $HfO_2$, and vice versa, determines the resistive property of the TMO.

## CONCLUSION

We have used first principles calculation based on DFT to propose a mechanism of resistive switching in a TMO-based RRAM. The proposed mechanism is based on the presence of continuously aligned oxygen vacancies with charge carrier trapping and its migration between the electrode-TMO interface and its bulk.

## REFERENCES

[1] R. Waser, and M. Aono, *Nanoionics-based resistive switching memories*, Nature Materials **6**, 833 (2007).
[2] P. Gonon, M. Mougenot, C. Vallée, C. Jorel, V. Jousseaume, H. Grampeix, and F. El Kamel. *Resistance switching in $HfO_2$ metal-insulator-metal devices.* Journal of Applied Physics **107**, 074507 (2010).
[3] S.M. Aspera, H. Kasai, H. Kishi, N. Awaya, S. Ohnishi, and Y. Tamai. *Realization of the Switching Mechanism in Resistance Random Access Memory™ Devices: Structural and Electronic Properties Affecting Electron Conductivity in a Hafnium Oxide-Electrode System Through First-Principles Calculations*. Journal of Electronic Materials **42**, 143 (2013).

978-3-901578-26-7 

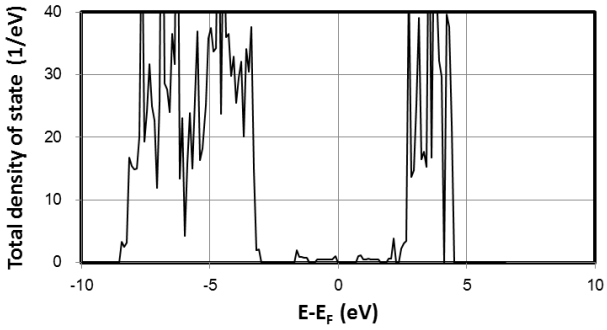


Fig. 1. Total density of states (TDOS) vs energy relative to the Fermi level (E-$E_F$) for bulk $HfO_2$ with rowed oxygen vacancies.

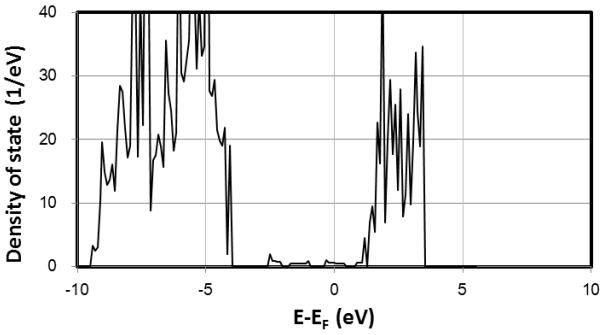


Fig. 2. Total density of states (TDOS) vs energy relative to the Fermi level (E-$E_F$) for bulk $HfO_2$ with rowed oxygen vacancies and charge carrier trapping.

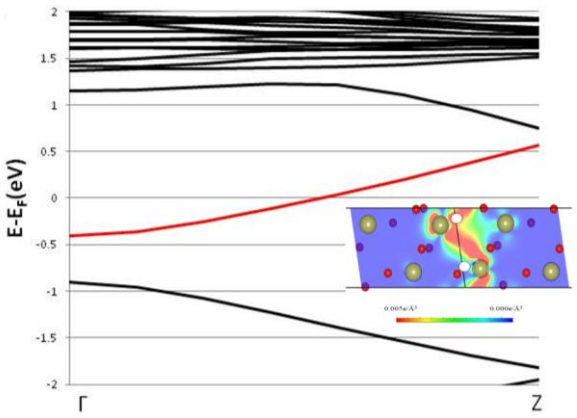


Fig. 3. Band structure plot near the Fermi level of bulk $HfO_2$ with rowed oxygen vacancies and charge carrier trapping. The highlighted red line shows the band passing through the Fermi level. *Inset*: partial charge density distribution plot for the band (shown in red) passing through the Fermi level. Green, red, and white spheres represents Hf atoms, O atoms and O vacancies, respectively. The colors indicate electron densities of until 0.005 e/Å$^3$.

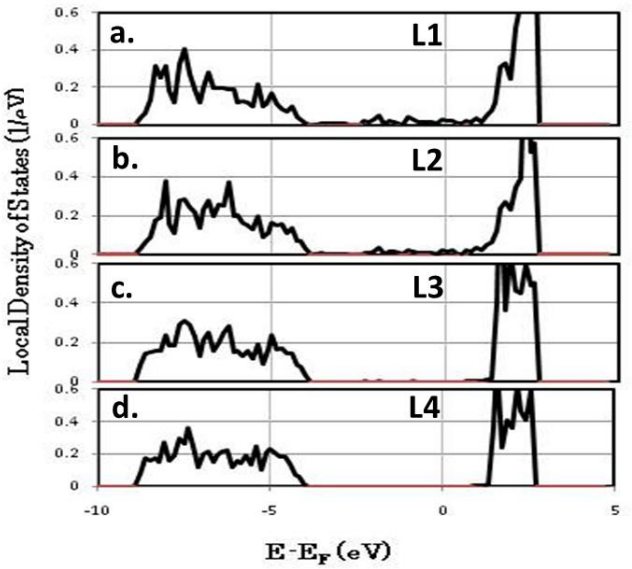


Fig. 4. Local density of states (LDOS) vs the energy relative to the Fermi level for $HfO_2$ layers (L1, L2, L3, and L4) near the electrode(Ta)-$HfO_2$ interface. L1 depicts the LDOS of the $HfO_2$ layer at the interface whereas L4 depicts the LDOS of the 4$^{th}$ layer of the $HfO_2$ bulk from the interface.

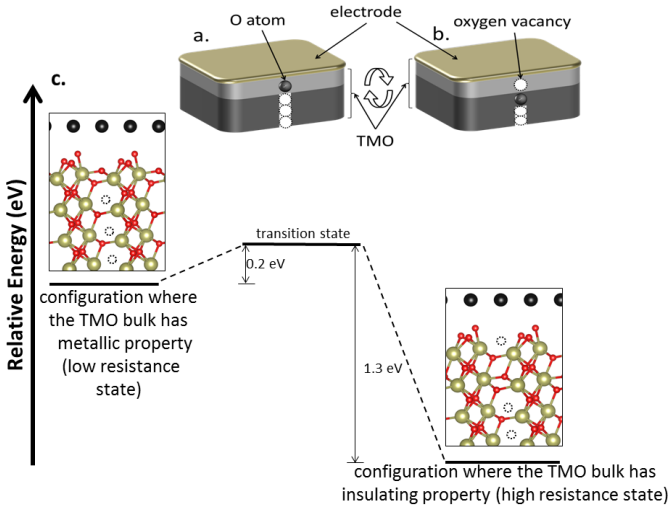


Fig. 5. Schematic illustration of the switching mechanism: a. high resistance state, b. low resistance state, and c. relative energies of the configuration with low and high resistance states, and the position of the transition state for oxygen vacancy migration. *Insets in Fig.5c*: configuration of the system. Green, red, white and black spheres represents Hf atoms, O atoms, O vacancies and Ta atoms, respectively.