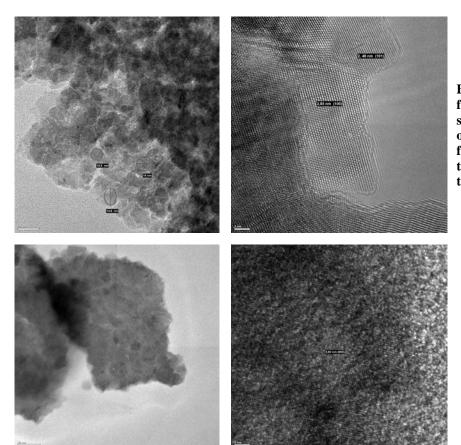
- Experimental studies on thin films semiconductor oxides deposition by solgel and DC/RF magnetron sputtering methods, for advanced optoelectronic and magnetic devices. Characterization of morphology, thickness, grains size, texture, structure, refractive index, transmittance, extinction coefficient, fluorescence properties and elemental composition.
- 1. Sn-Zn-O (Sn/Zn=1) thin films obtained by sol-gel route.
- 2. ZnO thin films and ZnO:Al doped thin films obtained by sol-gel route.
- 3. ZnO thin films deposited using DC and RF magnetron sputtering from Zn and ZnO targets.



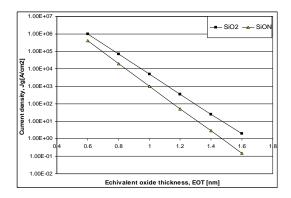
Bright Field HR-TEM images of ZnO thin film deposited by DC magnetron sputtering from Zn target and further oxidized in air at a temperature of 450°C for 3h. The nanocrystallites size is less than 20 nm, (100) and (002) oriented, and their structure is wurtzite.

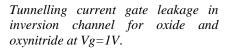
HR-TEM images of ZnO thin film deposited by RF magnetron sputtering from ZnO target. The grains size is less than 50 nm, (002) oriented nanocrystallites and wurtzite structure.

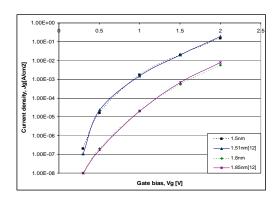
• Tunnelling leakage current characterization of silicon oxide and high-k dielectrics for advanced semiconductor devices.

Numerical simulations were performed using ATLAS devices simulator software package from Silvaco. An iterative approximate method was used to calculate the 1D MOS structures main electric parameters without using the Schrödinger-Poisson

equations. This method is based on approximation of effective field function of doping parameters. The tunnelling currents can be calculated more rapidly and the study for different gate dielectric stacks can be made.



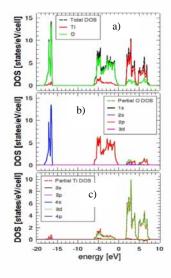


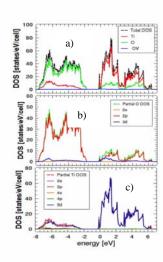


Calculated data and experimental gate leakage currents for high-k stacks with Al_2O_3 .

• Ab initio study of electronic structure of semiconducting oxides. Modelling of defects influence on localized states.

Ab initio calculations were performed using the FPLO code in order to explore the electronic structure of semiconductor oxides for advanced opto- and magneto-electronic devices. The oxygen deficiency in these materials may be used to tune the material optical and magnetical properties. The computational study was devoted to understand the effect of oxygen vacancies (OVs) on the electronic structure of rutile and anatase TiO₂. Various OVs concentrations and distributions in the supercell permitted to determine the vacancy-induced states localization and structure, the effect of vacancy concentration on the orbital occupation numbers, as well as the vacancy energetics. The present results, reflect the real material behavior.





Total and element-projected DOS, a), Partial and angular momentum-projected O DOS, b) and Partial and angular momentum-projected Ti DOS, c) of stoichiometric rutile TiO₂. The Fermi level is at 0 energy.

Total and element-projected DOS for 6.2 % OVs distributed as: isolated vacancies a), OVs arranged as isolated pairs with perpendicular b) and parallel orientation c) to the crystallographic c-axis. The Fermi level is at 0 energy.