AB INITIO STUDY OF HIGH PERMITTIVITY HF OXIDES FOR CMOS NANOELECTRONIC

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In the downscaling context, the MOS transistor dimensions shrink regularly. In order to follow the ITRS road map, the gate oxide has to be replaced (to avoid leakage current) by a new material with a high permittivity called « high-k » material (in order to thicken oxide keeping the property of the capacity). During the last few years the new material which has shown the most interesting properties is the hafnium dioxide (HfO_2). However the use of this new MOS stack involves new challenges, namely concerning the comprehension of its electronics properties. The scale of the devices being of the order of a nanometer, it becomes interesting and necessary to study this new stack with an atomistic approach using ab initio methods. The ab initio methods we are using rely on the density functional theory (DFT[1,2]). Mainly, the abinit program www.abinit.org has been employed.

Firstly our study purpose has been to reproduce the material structure existing in a MOS stack. Several publications [4,5] have shown the cubic, the tetrahedral and the monoclinic structure for HfO_2 bulk material. But, experimentally, the phase caught in a thin MOS stack is polycrystalline including the monoclinic and orthorhombic phases. So, we tried and succeed to obtain those 2 phases separately, by DFT/LDA energy minimization techniques.

Besides, we have already obtained the band structure of monoclinic HfO2, with DFT density functional theory and then we corrected it with the GW approximation [3] in order to get a band gap in good agreement with experiment. The value of the GW corrected band gap we obtained is 7.1 eV. This is in good agreement with a band gap of 6.7 eV, recently obtained by a mixed computational (DFT) and experimental approach [7]. (Let's recall that the GW approximation take into account electrons interactions within a perturbative many body approach which is not possible simply using DFT).

Following that, we will soon obtain the band structure of metal gate and then we will be able to simulate the whole structure of a nanometric MOS stack, in order to study the band alignment between a chosen metal and a highK material and the associated effective work function, which is critical for the future nanoelectronic devices.

References:

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Figures:

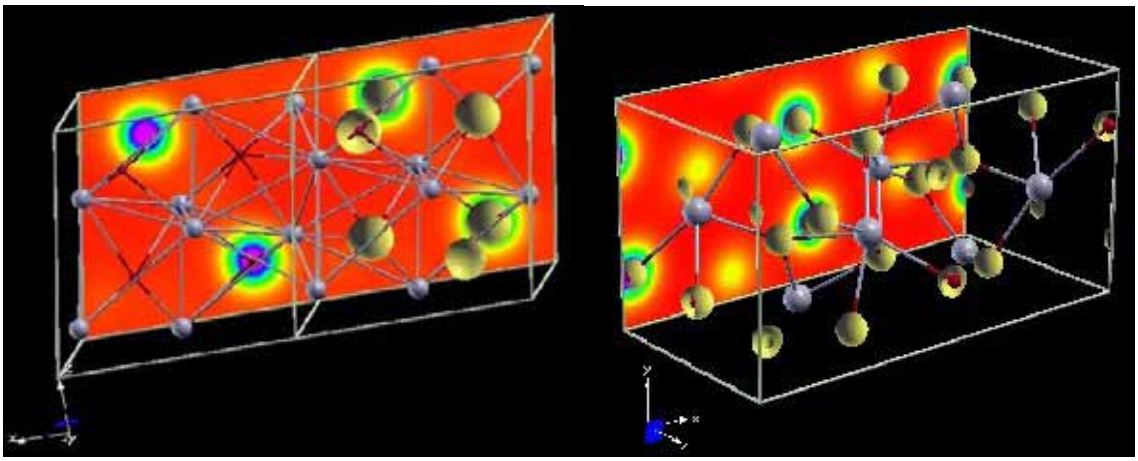

Fig. 1: HfO_2 monoclinic and orthorhombic phases, showing electronic contours (XCrysden [6]).

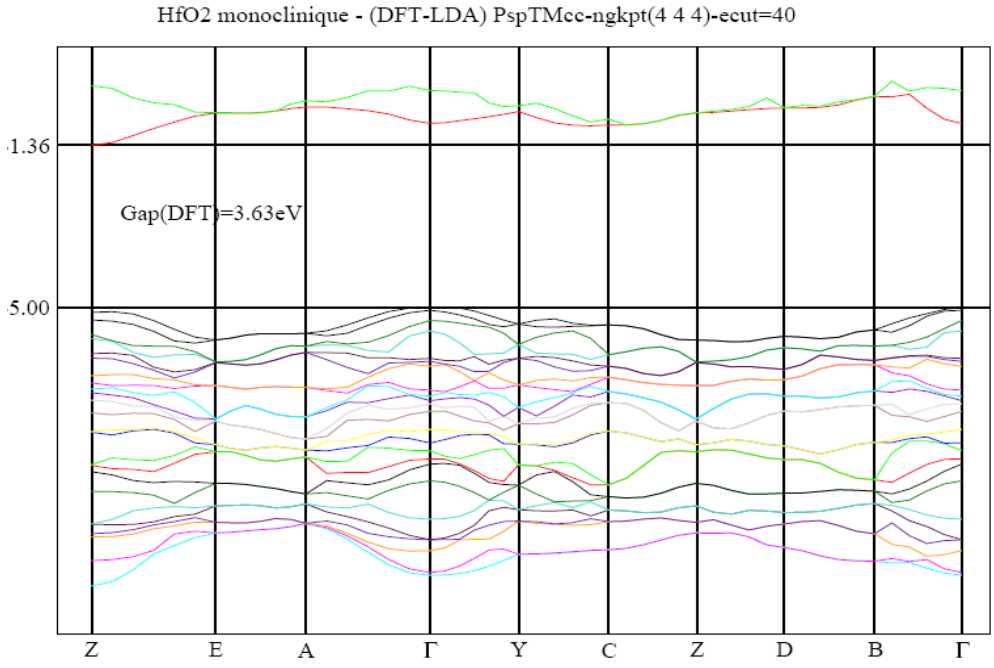

Fig. 2: HfO_2 monoclinic DFT band structure with a 3.63 eV indirect band gap ; the GW corrected band gap value for the same phase value is 7.1 eV.