



**Friday-February 24, 2017**

**12:00-1:00 PM**

**BECTON SEMINAR ROOM**  
**Light lunch will be served at 11:45 a.m.**

**Mehmet Dogan**

Applied Physics Department, Yale University  
P/I Prof. Sohrab Ismail-Beigi

***Ab initio* Study of HfO<sub>2</sub> Thin Films**

Recent discovery of HfO<sub>2</sub>-based ferroelectric thin films makes it possible to realize one-transistor memory cells that offer attractive features such as low power, high speed, small cell size, scalability and CMOS compatibility. As is demonstrated by different experimental characterization methods, ferroelectricity in HfO<sub>2</sub> arises from the creation of a polar orthorhombic phase (space group: Pca2<sub>1</sub>) that is generated during the rapid annealing process with the help of a suitable capping electrode. This electrode (typically TiN) provides the confinement that is believed to be essential in the formation of the polar phase. It has also been demonstrated that the polarization in HfO<sub>2</sub> thin film is affected by different fabrication conditions, such as doping species and doping concentration in the oxide, annealing temperature, film thickness etc. Some of the effects of these factors on the film polarization are not yet fully understood. Because the relative ratio of the orthorhombic phase over the non-polar phases determines the functionality of FE-HfO<sub>2</sub> devices, a thorough understanding of what decides this ratio is crucial in optimizing the growth procedure that yields the best performing oxide film. To this end, in this *ab initio* study, we investigate the energetics of different bulk phases of HfO<sub>2</sub> with varying amounts of Si and Zr doping and different epitaxial strain states. These results, together with additional analysis, help explain the common experimental observations as well as some of the underlying causes from an atomic structure viewpoint. We also describe preliminary results on simulated HfO<sub>2</sub> thin films including the interface with the electrode to get a more comprehensive understanding of the energetics in thin films.

**Nanbo Gong**

Department of Electrical Engineering, Yale University  
P/I Prof. T.P. Ma

**Ferroelectric Memory: A Re-Emerging Technology Poised to Take Over DRAM or Flash Memory**

Ferroelectric-gated Field-Effect Transistor (FeFET) was shown to be capable of storing binary information as early as in the 1960's. Unfortunately, FeFET-based memory technology has not yet succeeded in commercialization despite intensive R&D efforts for decades and its numerous theoretical advantages compared to the dominating nonvolatile memory technology (flash memory), including programming speed, power consumption, and endurance. The key stumbling block for commercialization has been the lack of suitable ferroelectric materials that enable fabrication of FeFETs to fulfill the requirements for a viable memory technology, including memory retention, CMOS compatibility, and scalability.

The recent discovery of HfO<sub>2</sub>-based ferroelectric has changed the outlook of the FeFET-based memory technology, and it is now widely believed that it has re-emerged as the memory technology that will most likely take over the currently dominating flash memory. In this talk, I will introduce the principle of operation of the FeFET memory, its advantages compared to its competitors, the problems of the "pre-HfO<sub>2</sub>" ferroelectrics (such as PZT and SBT), the key to the formation of the HfO<sub>2</sub>-based ferroelectrics, the special attributes of ferroelectric HfO<sub>2</sub> for the FeFET memory technology, and some related research contributions that our group has made.

**Host: Professor Eric Altman**