Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic properties of oxygen vacancy in HfO_2 within GW calculations EUN-AE CHOI, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea — Hafnia (HfO_2) has attracted much attention as a high-k dielectric material, which substitutes for silicon gate oxide in nanoscale metal-oxide-semiconductor (MOS) devices. However, there remain several problems to be resolved in hafnia-based devices, such as flat band shift and threshold voltage instability. Oxygen vacancy, as the most common intrinsic defect, is regarded as a major cause of these problems. As previous calculations mostly rely on the local-density-functional approximation (LDA), the defect levels of oxygen vacancy are not accurately determined because of the LDA band gap problem. Here we perform GW calculations for the defect levels of oxygen vacancy in monoclinic HfO_2. Our calculations show that the Fermi level pinning of p+ poly Si gate electrode is due to the charge transfer from oxygen vacancy to the electrode. In addition, the charge trap of oxygen vacancy can lead to the threshold voltage instability in both nMOS and pMOS devices. Finally, we suggest that oxygen vacancy may be a cause of the gate leakage current by the Poole-Frenkel conduction.

Eun-Ae Choi
Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea

Date submitted: 01 Dec 2008 Electronic form version 1.4