Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

**Oxygen vacancies in amorphous-$Ta_2O_5$ from first-principles calculations**[1] JIHANG LEE, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan, WEI LU, Electrical Engineering and Computer Science, University of Michigan — Oxygen vacancies are thought to play a crucial role in the electrical and optical properties of tantalum pentoxide ($Ta_2O_5$) devices. Even though numerous experimental studies on oxygen vacancies in $Ta_2O_5$ exist, experimentally detected defects are ambiguously identified due to the absence of an accurate and conclusive theoretical analysis. We investigate oxygen vacancies in amorphous $Ta_2O_5$ with first-principles calculations based on hybrid density functional theory. The calculated thermodynamic and optical transition levels of stable oxygen vacancies are in good agreement with measured values from a variety of experimental methods, providing conclusive clues for the identification of the defect states observed in experiments. We determine the concentration of oxygen vacancies and their dominant oxidation state as a function of growth conditions. We analyze the characteristics of extra electrons introduced by donor-like oxygen vacancies, which include the formation of polarons. Our results provide insight into the fundamental properties of oxygen vacancies in $Ta_2O_5$, which is essential to controlling the properties of films and optimize the performance of devices.

[1]This research was supported by the AFOSR through MURI grant FA9550-12-1-0038 and the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational resources were provided by the DOE NERSC facility.

Jihang Lee
University of Michigan - Ann Arbor

Date submitted: 06 Nov 2015 Electronic form version 1.4