Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Oxygen vacancies in monoclinic hafnia[1] MANISH JAIN, University of California, Berkeley, Lawrence Berkeley National Laboratory and University of Texas, Austin, JAMES R. CHELIKOWSKY, University of Texas, Austin, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — Hafnia has recently received much attention because of its potential application as high-dielectric material replacing silica in microelectronic devices. Point defects – in particular oxygen vacancies – play an important role in this material as electron or hole traps. In this study, we perform electronic structure calculations on oxygen vacancies in hafnia using a combined Density functional Theory (DFT) and GW/BSE formalism. This formalism corrects for the error in calculating formation energy and charge transition levels using standard DFT. While there have been some GW studies on oxygen vacancies in hafnia using small supercells, we perform calculations using large supercells with 96 atoms. Such a large supercell calculation should minimize any spurious defect-defect interactions.

[1]This work was supported by National Science Foundation Grant No. DMR07-05941, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 and DE-SC0001878. Computational resources have been provided by NSF through TeraGrid resources at TACC.

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Date submitted: 19 Nov 2009 Electronic form version 1.4