Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Carbon clusters as possible defects at the SiC-SiO_2 interface[1]
YINGDI LIU, HONGLI DANG, YANG LIU, YING LI, University of Tulsa, MATTHEW CHISHOLM, Oak Ridge National Laboratory, TRINITY BIGGERSTAFF, North Carolina State University, GERD DUSCHER, University of Tennessee, Knoxville, SANWU WANG, University of Tulsa — High state densities in the band gap of the SiC-SiO_2 interface significantly reduce the channel mobilities in SiC-based high-temperature/high-power microelectronics. Investigations of the nature of the interface defects are thus of great importance. While several possible defects including very small carbon clusters with up to four carbon atoms have been identified by first-principles theory, larger carbon clusters as possible defects have attracted less attention. Here, we report first-principles quantum-mechanical calculations for two larger carbon clusters, the C_{10} ring and the C_{20} fullerence, at the SiC-SiO_2 interface. We find that both carbon clusters introduce significant states in the band gap. The states extend over the entire band gap with higher densities in the upper half of the gap, thus accounting for some of the interface trap densities observed experimentally.

[1]Supported in part by the NSF (CMMI-0645953), by the Oak Ridge Associated Universities, by the National Center for Supercomputing Applications (TG-DMR080005N), and by the National Center for Computational Sciences at Oak Ridge National Laboratory.

Sanwu Wang
University of Tulsa

Date submitted: 21 Nov 2008 Electronic form version 1.4