

Physics Colloquium

Michigan Technological University

April 21 (Thursday) 2005, 4:00 to 5:00 pm
Room 139, Fisher Hall

Electronic Structure of Point Defects in SiO₂

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Amorphous SiO₂ has served as the gate dielectric material of choice in conventional microelectronics since the inception of the industry. Point defects present from manufacture or generated from exposure to the space radiation environment have effects that limit the lifetime of space-based electronics. Defects generated in the bulk of the material generate conduction paths that result in transistors being left permanently in one state. Defects generated at Si/SiO₂ interfaces also lead to charging effects that change the current/voltage characteristics of a device. Because of the amorphous structure of the material, the structural properties of these defects are difficult to characterize. Even now as amorphous SiO₂ gives way to more exotic materials in terrestrial and space applications, the structure of some of these defects remains controversial. One of a family of oxygen-related defects is the so-called E'₈ center. Recent experimental evidence has called into question our group's interpretation of this defect as an oxygen vacancy in which an unpaired electron is delocalized over a pair of Si atoms.

In this colloquium, I will review the electronic structure calculations which lead us to this interpretation and the new results that have called this interpretation into question.

Andrew C. Pineda is a Senior Research Scientist at the University of New Mexico (Department of Chemistry and Center for High Performance Computing). A native of Arizona, he received a B.S. degree in Chemistry from Harvey Mudd College (Claremont, CA). At Harvard University, he studied enhanced fluorescence and energy transfer properties of micron-scale objects, receiving the M.A. in 1984 and Ph.D. in Physical Chemistry in 1994. After a brief period in the computer industry, he joined the Center for High Performance Computing at UNM in 1997 and is now based out of the Department of Chemistry. Much of his work has focused on utilizing the methods of electronic structure theory to understand the properties of radiation-induced defects in semiconductor materials. His current research interests include III-V materials and high-k dielectrics.