Department of Electrical and Computer Engineering

Cluster Hire in Computational Aspects of Multiscale Materials Modeling

Faculty Candidate Seminar

Density functional theory for CMOS technology

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260 Dreese Laboratory
2015 Neil Avenue

As scaling of the complementary metal oxide semiconductor (CMOS) technology takes us below 65 nm many new materials, traditionally not associated with the semiconductor process, are being introduced into manufacturing. Notably, transition metal (TM) oxides or more generally dielectrics with a high dielectric constant or high-k dielectrics will be used for the gate stack applications instead of SiO2. After the introduction of Cu this is arguably the most drastic departure from the traditional CMOS process. The physics and chemistry of these materials is much more complicated than that of Si3N4 or SiO2, and theoretical calculations of their properties have proven to be extremely useful in both process development and device engineering. The work horse of the modern computational materials science is density functional theory (DFT) within the local density approximation (LDA) and pseudopotential (PP) approximation. In this talk I will focus on the recent theoretical work performed in my group on problems of interfaces, band alignment and transport characteristics in gate stacks containing TM oxides.

Ironically, the introduction of non-Si based oxides may spell the end of silicon's dominance of electronics. I will comment on materials issues for CMOS beyond silicon.

Alex Demkov received his Ph.D. in 1995 at Arizona State University, and stayed on at ASU as a postdoc. In 1997 he joined Motorola's R&D organization working both in Semiconductor and Corporate Research Labs. He joined the faculty at the University of Texas at Austin in 2005. Demkov co-authored over seventy research papers and holds five US patents. His group conducts theoretical research in the area of electronic materials and quantum transport. In 2006 Demkov received the NSF CAREER Award and was elected Fellow of the American Physical Society for his work on the theory of materials for advanced CMOS.