



# TEXAS ADVANCED COMPUTING CENTER

THE UNIVERSITY OF TEXAS AT AUSTIN

## General Info

- [Home Page](#)
- [TACC Overview](#)
- [Staff](#)
- [New Users](#)
- [Press & Events](#)
- [Affiliations](#)
- [Contact Info](#)
- [Visitor Info](#)
- [Employment](#)

## Resources

- [HPC Systems](#)
- [Visualization](#)
- [Data Storage](#)
- [Networking](#)
- [Software & Tools](#)
- [Allocations](#)
- [Usage Policies](#)

## Services

- [User Portal](#)
- [User Guides](#)
- [User News](#)
- [Consulting](#)
- [Training](#)
- [Cluster Support](#)
- [EOT](#)

## Research/Development

- [TACC Projects](#)
- [TACC Publications](#)
- [User Research](#)
- [SciVis Gallery](#)
- [Industrial Partners](#)
- [Petascale Lecture Series](#)
- [International Partners](#)

## Focus Areas

- [HPC](#)
- [SciVis](#)
- [DIS](#)
- [Dist./Grid Computing](#)

## Search

## Designing the Nanofuture

TACC supercomputers help Alex Demkov devise tomorrow's semiconductors

It's practically a given that this year's PCs will be significantly faster than last year's and that each supercomputer will blaze past its predecessor. This trend in computer hardware, dubbed Moore's Law, depends primarily on engineers' ability to miniaturize transistors and double the number that can be placed on an integrated circuit every two years. However, scientists recently discovered that at the 32-nanometer scale — the current target for semiconductor fabrication — the behavior of the materials used to make transistors changes in distinct and unexpected ways.

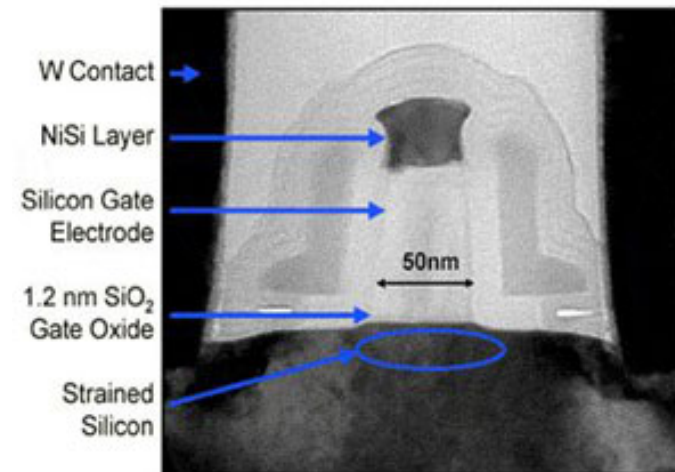
"It's called quantum tunneling," Dr. Alex Demkov, professor of physics at The University of Texas at Austin, explained. "These are basically mundane transistors, but the reason they can't operate at such a thickness (32nm gate lengths require sub-nanometer gate dielectrics) is that, at the smallest scales, electrons have the ability to behave like waves and to tunnel under barriers."

The tunneling causes electrical charges — the driver of computer power — to leak through the gate dielectric, making the mechanism ineffective. So a search began among chipmakers and researchers for new processes, new architectures, and new, unexplored materials to continue shrinking the transistor.

Demkov is at the forefront of this search. Investigating materials for what is known as the gate stack — the most important element of a transistor's speed — his research bridges the gap from first principles to device physics, and helps uncover the rules that govern the production and operation of working computers and cell-phones.

**Prompted by the tunneling leakage problem, the industry converged on an oxide of a semi-obscure element,**

Prompted by the tunneling leakage problem, the industry converged on an oxide of a semi-obscure element, hafnium, as the basis for nano-scale semiconductor technology, stimulating new



Transmission electron microscopy image of a 65 nm semi-conductor.

## **hafnium, as the basis for nano-scale semiconductor technology, stimulating new questions about an old material.**

degrees, it turns out that no one knows what's going to happen. So we try to understand material properties in the context of high-purity, high-tech manufacturing."

Though it is possible (and necessary) to test new, semi-conducting materials in the lab, the process is too time-consuming for the optimization of hafnium compounds in manufacturing. To speed the search, Demkov relies on the Lonestar high-performance computing system at the Texas Advanced Computing Center (TACC). "TACC has been very good to us," Demkov said. "My group burns over a million SUs [computing hours] a year, so we are a very large consumer of TACC's resources."

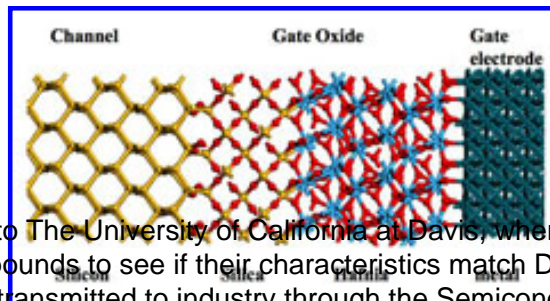
This collaboration between academic scientists and HPC centers ends up helping the semiconductor industry as well. "Supercomputers have allowed us to move from performing calculations on single materials — understanding a large piece of silicon — to device structures — for example, a complete stack — without compromising accuracy," said Stefan Zollner, an engineer at Freescale Semiconductor and a collaborator of Demkov's. "Without supercomputers, we would need empirical rules on how to match bulk properties at interfaces when building device structures, or we would have to give up accuracy and perform less-accurate simulations with empirical force fields."

The immense computational power of supercomputers like Lonestar enables Demkov to explore the characteristics of novel compounds. "Can you predict the atomic structure or the crystalline structure of these materials? If you can, you can tell how that translates into electrical properties," Demkov explained. "It's quantum mechanics meets metallurgy."

questions about an old material. "When you look at a material like hafnium dioxide (HfO<sub>2</sub>), you say, 'Everything is known about it,' and that's true," Demkov explained. "But when you lay down a film which is only forty angstroms [0.4 nanometer] thick and place it on a silicon substrate and put in a metal gate and heat the substance to one thousand

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As a theoretician at work on real world problems, Demkov collaborates with experimentalists to develop new materials for production use. He is currently working on a joint project with graduate student, Xuhui Luo, that uses quantum mechanics to simulate the behavior of materials with a high



sent to The University of California at Davis, where a third team (led by Prof. A. Novrotsky) analyzes the compounds to see if their characteristics match Demkov's predictions. The insights from the process are then transmitted to industry through the Semiconductor Research Corporation, where they shape future production methods.

*Ball-and-stick diagram of a hafnia gate-stack. Image courtesy of Onise Shariq, The University of Texas at Austin.*

dielectric (high-k) constant, meaning they polarize in reaction to an applied electric field. His collaborators at The University of Texas at Austin Chemical Engineering department (led by Prof. J.G. Ekerdt) synthesize the most promising computationally-derived materials in a lab. Then, these materials are

The collaborative process allows labs with different capabilities to work together, revise, and hone each part of the procedure based on the feedback of their colleagues, speeding the discovery of usable materials for semi-conductors. Just as importantly, Demkov says, the process provides his graduate students with a chance to learn how products are developed in commercial laboratories.

"I'm often asked, 'What is your deliverable?' I answer that my deliverable is a graduate student, a trained professional who will move the economy for the next twenty years," Demkov said. "Only 10% of Ph.D. students become professors. The rest of them will work in the real world, and the real world is very interdisciplinary. You never have all the information, and you have to make decisions fast. Working on this project, they get an experience that will serve them well in the future."

Demkov's investigations into hafnium dioxide are just one of the projects in his research portfolio. Long-range projects involve applying computational physics to biology to examine the quantum mechanical basis for photosynthesis, aerobic respiration and vision, as well as designing smaller and better mechanisms for use in information technology.

When TACC's newest petascale computing system, Ranger, goes into full production in January 2008, Demkov believes the capability will finally exist to design nanoscale devices through massively parallel simulations. "If you want to describe a functional element of a transistor, you need only about five hundred to a thousand atoms. With the help of supercomputing systems at TACC, you can do this from first principles," Demkov said. "You can actually build an atomic structure which, when you step aside, would look like a real device."

**"The question is, can you predict the atomic structure or the crystalline structure of these materials? If you can, you can tell how that translates into electrical properties," Demkov said. "It's quantum mechanics meets metallurgy."**

Through partnerships like those between Demkov and TACC, the next generation of computers will continue to leave today's technology in the dust, satisfying Moore's law and driving the innovations of tomorrow.

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