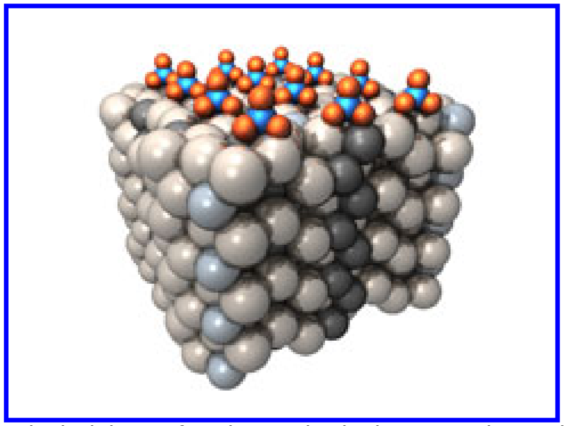
TEXAS ADVANCED COMPUTING CENTER
THE UNIVERSITY OF TEXAS AT AUSTIN

Sailing the Uncharted Seas of Materials Discovery

Dr. Stefano Curtarolo teams with TACC to explore new materials

“One gram of practice is worth more than a ton of theory,” Dr. Stefano Curtarolo declares, “so as a theorist, I always look for practical applications.” Curtarolo, assistant professor of materials science at Duke University, studies the properties of novel and theoretical materials using computational methods. However, it is not the abstract knowledge that drives Curtarolo’s research, but the real world inventions that result from his simulations: hand-held nuclear particle detectors for homeland security; nano-catalysts to reduce fossil fuel emissions; and new methods to find tomorrow’s superconductors.



"Hypothetical" layer of methane adsorbed on a quasi-crystalline surface

Curtarolo has studied the properties of elements and small structures for more than a decade. In that time, he has seen incredible strides in the field, many of them made possible by advances in supercomputing.

“Materials are made of atoms and unless you are studying a system with only four or five atoms, anything more requires a supercomputer to help you,” Curtarolo explained. “Experimentalists need big labs and expensive microscopes, but theoreticians need big computers with a lot of CPUs, a lot of memory and a lot of bandwidth.”

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Curtarolo uses the Lonestar system at The Texas Advanced Computing Center (TACC) — currently #22 on the Top500 list of the world's fastest supercomputers — for his disparate material property research problems. His explorations of carbon-tube catalysts, super-alloys, quasi-crystal structures and superconductors netted Curtarolo career awards in 2007 from the Navy and the National Science Foundation, and led to the prediction of a superconducting, lithium-boron "sandwich." But he couldn't do it on his own.

"Materials are made of atoms and unless you are studying a system with only four or five atoms, anything more requires a supercomputer to help you," Curtarolo explained. "Experimentalists need big labs and expensive microscopes, but theoreticians need big computers with a lot of CPUs, a lot of memory and a lot of bandwidth," he said.

"Without TACC, I would be in trouble," Curtarolo admitted. "I would do fewer computations, fewer projects, and projects of lower quality. When you're able to simulate bigger systems, your results are going to be more accurate. Without a precise description of the system, sometimes you're not even capable of understanding a particular phenomenon."

Our high school chemistry classes might have led us to believe that the weight, density and resistivity of materials were well established. However, when scientists look beyond the bulky macroscopic characteristics of materials down to the nano-level — structures as small as one nanometer, or roughly one thousand times smaller that the width of a human hair — they often find material characteristics far different than those they expected, with strange and potentially useful states.

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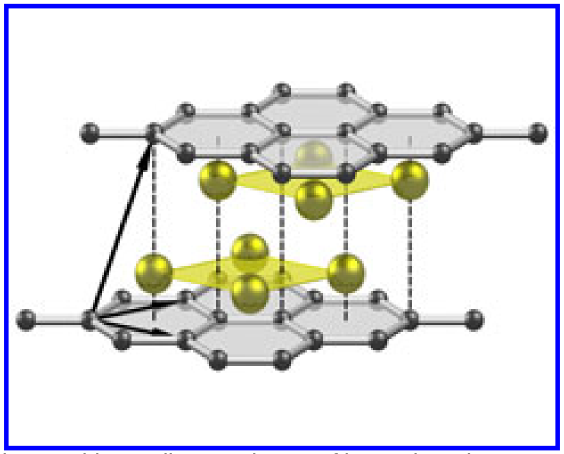
"Going from macro to nano completely changes the physics of the systems," Curtarolo explained, "but so far, we've only been able to calculate the properties of very small systems, ten to one-hundred atoms maximum. This is why we need supercomputers, because by increasing the size of the calculations, we can see phenomena that happen only on the nanoscale that are worth investigating." Curtarolo recently completed a paper using a quantum mechanics simulation of up to three hundred-atoms, among the largest nanoparticles calculated to date.

Nanotechnology has significant potential not only in computing, but also in medicine, alternative energy production and engineering. However, supercomputers themselves cannot resolve the nature of nanostructures. "It's not just a matter of computer speed. It's also knowing how to use supercomputers," Curtarolo said. "Some of the codes that we use, and some of the ideas we develop, are really complicated and require people with a lot of creativity to phrase them in the right way. We need to start thinking more about how to use these computers in the best possible way, because their power is enormous. Never in human history have we had the capability of using such big machines."

For Curtarolo, who uses approaches and ideas from multiple fields to direct his research, science is open-ended and interdisciplinary. His investigations span four major research areas, including the qualities of alloys; the stability of nano-structures; superlubrication in quasi-crystals; and the detection of nuclear particles. Amazingly, Curtarolo's most significant discovery happened accidentally, when he stumbled on the lithium-boron metal-sandwiches while doing theoretical materials research for another project.



In the new binary alloy, two layers of boron 'bread' surround a 'filling' of lithium metal.

"I developed the method of data-mining quantum calculations to correlate crystal structures energy and generate predictions in new systems. Aleksey Kolmogorov [a former postdoctoral associate] and I were using that method to study magnesium alloys to make better cars, and we ended up finding the superconductor lithium-boron, which we were not looking for," Curtarolo said.

The prediction came with the application of "ab initio" (from first principles) methods to materials science. This method allows high-performance computing systems to predict and characterize the structure of materials by simulating the properties of a material based on its atomic components and the laws of electrodynamics. By parallelizing his code for Lonestar, Curtarolo was able to complete 900,000 hours of computing time on 670 jobs (across almost 10,000 allocated cores) in nine months.

In addition to his research into specific materials, Curtarolo has developed new methods to improve the way scientists use and share their findings. Like many others, Curtarolo recognized that the proliferation of research was causing scholars to repeat existing studies as they struggled to keep up with the literature within their subfield. The underutilization of existing research inspired Curtarolo to develop a unique method of computational analysis that combines ab initio methods of material investigation with data mining of past quantum equations to speed the pace of material knowledge. Rather than reinvent the wheel, this method uses the results of thousands of

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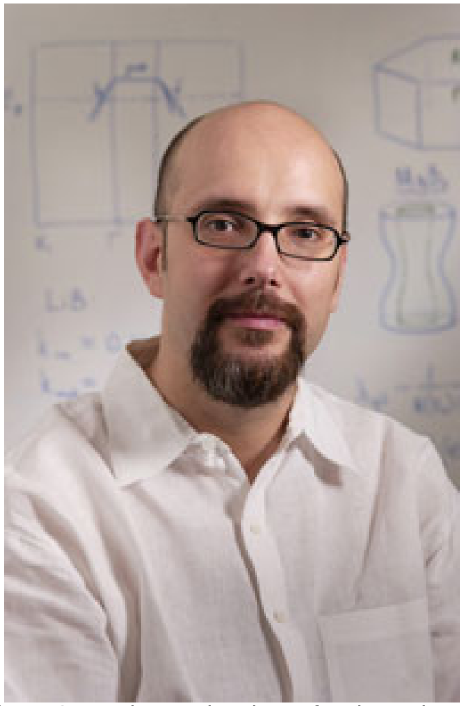
previous simulations to theorize the crystal structure of known and unknown materials.

the results will be."

"Supercomputers are becoming so powerful, but they'll never be able to think like a human," Curtarolo said. "We are already capable of calculating many materials properties, but by training supercomputers with very smart algorithms, we might be able to devise materials with the requested properties. So I try to develop good methods and good codes that allow the computers to search for materials by themselves. Instead of finding one 'lithium-boron system' every three years, I want to make a code that generates hundreds of those. And the supercomputer should be smart enough to understand if the systems are worth studying or not."



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If his work is successful, Curtarolo will help usher in an era of smart discovery, where supercomputers predict nanostructures and superconductors with the potential to solve grand challenge problems.

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To follow Dr. Curtarolo's research and discoveries, visit his homepage: http://www.mems.duke.edu/faculty/curtarolo/.

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