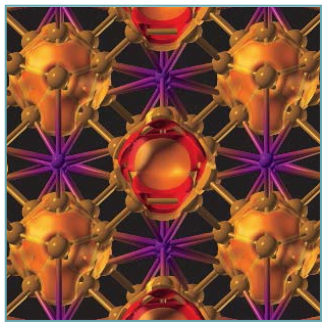
Faculty Profile:

Artem R. Oganov Leads the Way in Computational Crystallography

Greetings to Geoscience friends and alumni! I moved to Stony Brook in November 2008 and have found it to be a wonderful place to live and work. One day, when I have nothing better to do, I'll write a book of memoirs, but for now let me tell you my story and a bit about my research and teaching.

I was born in Moscow, Russia, in 1975. Our family is very large and diverse — among my relatives are engineers, artists, programmers, business people, doctors, lawyers, politicians, soldiers, teachers, musicians, pilots; they live in nine different countries and speak seven languages. Since the age of six I dreamed of becoming a chemist, and from the age of seven attended chemistry lectures at Polytechnic Museum and University of Chemical Technology. With time my interests evolved – first to mineralogy, then to physics. But I always knew that I would be a scientist. In 1997 I graduated from Moscow State University with an MSc degree in Crystallography, and, having obtained a Russian Presidential Scholarship for Education-Abroad and a British Government Scholarship, I went to the U.K. I was fortunate to have Prof. David Price, a wise and inspiring person, as my supervisor. In early 2002 I obtained a PhD in Crystallography at University College London, and continued for 1 year as a postdoc. After that I took up a position of Senior Scientist at ETH Zurich, Switzerland. My mission was to organize a group in computational crystallography. This was a very successful experiment, and also great fun. In continental Europe there is a degree higher than PhD – it's called Habilitation. Mainly for fun, I obtained this degree in 2008. Later that year I came to Stony Brook. As it turned out, some of my relatives had also moved to Long Island. Not only Long Island, but also the Department has become a family-like environment.



Electronic structure of γ B28, a new phase of boron discovered at SBU

Here in Stony Brook, I've built a computational crystallography and mineral physics laboratory. We work on a diverse range of problems, from developing new simulation methods to computational materials design and to high-pressure mineralogy and physics. My teaching, both on undergraduate and graduate levels, focuses on these topics.

Prof. Artem R. Oganov

I keep on adapting my teaching strategies, to maximize the effectiveness of learning. I enjoy teaching almost as much as I enjoy research. The central question of my research is how the structure of matter relates to its properties, and how to predict both. The keys to success of my lab are strict selection of students and postdocs, family-like atmosphere and a lot of fun and play at work. Science is not only hard work, it is also fun! Our "toys" are some of the world's biggest supercomputers in the US and in Russia.

Let me mention a few of my research projects. In 2001 I figured out how to accurately compute the elastic constants of crystals at high temperatures, and performed the first calculations of this kind. From these it emerged that there are very large temperature variations in the Earth's mantle, reaching some 2000 K in its lowest part. In 2004, in collaboration with S. Ono (Japan), I found an explanation of the complex and counterintuitive properties of the Earth's D" layer, the lowermost part of the mantle. These properties are explained by a new silicate mineral, $MgSiO_3$ post-perovskite, that was found in our theoretical and experimental study, as well as in the simultaneous experiments done in Japan. Subsequently, in 2005 we discovered a similar phase of Al_2O_3. The same year, I proposed a mechanism of the phase transition leading to post-perovskite, and a mechanism of its plastic deformation in the mantle. In parallel, I worked with my graduate student Colin Glass, on solving the problem of crystal structure prediction. Widely believed to be insoluble, the problem of finding the most stable arrangement of atoms for a given chemical formula actually turned out to be amenable with the evolutionary algorithm that we have developed. The simulation code, initially written by Colin and later expanded by Andriy Lyakhov, is now used by almost a hundred researchers worldwide. Using this method, and in collaboration with many experimentalist and theoreticians (most notably, Yanming Ma, Vladimir Solozhenko, Mikhail Eremets, Jiuhua Chen), we made several exciting findings in the fields of high-pressure chemistry and physics. These included tetrahedral carbonate ions, a remarkable high-pressure superconductivity in GeH_4, a transparent form of sodium, and a partially ionic allotrope of boron with a rocksalt-type structure. Very recently, my old friend Mario Valle (Switzerland) and I worked on a new language for chemistry – the language of energy landscapes. This transforms chemical concepts into multidimensional spaces, and during this study we had to learn about hyperdimensional geometry, data mining and lots of other interesting things. My principle is not to limit creativity by artificial boundaries, but to solve any important problems that I can, and to learn from research. There is a lot to be done in all the fields of science related to the structure and properties of materials. And it is a pleasure to pursue this research at Stony Brook.

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