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Issue: ***February 2009***

A New Form of the Fifth Element

by Jessica Tanenbaum

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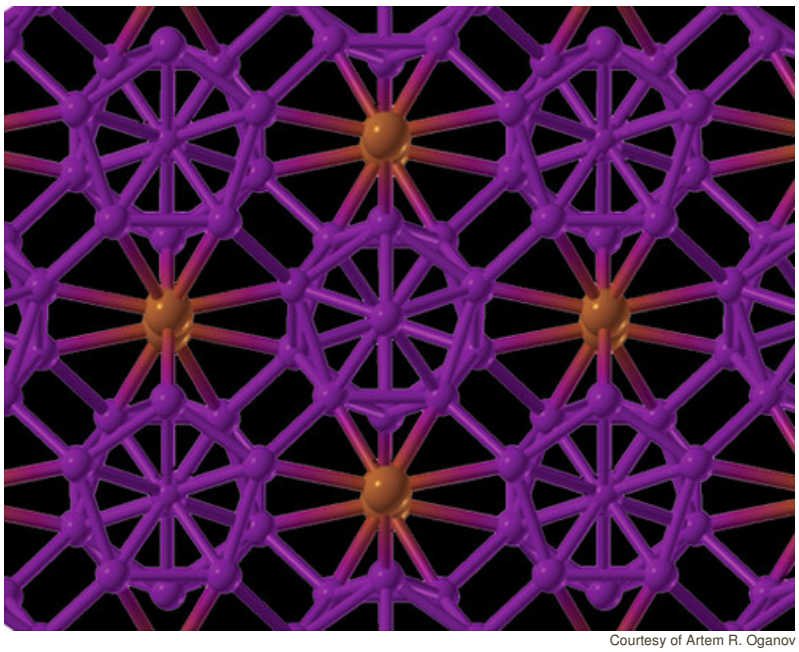
When two identical atoms form a bond, does only one atom snatch the bonding electrons, or do the atoms share?

Even if you're a chemistry newbie, you probably can guess that the atoms share the electrons — they form a covalent bond. It's only logical that identical atoms attract electrons identically. There's no reason for only one atom to get electron access. Except that this reasoning is not always true.

According to a new study published in the journal *Nature*, boron atoms bonded into molecules can form ionic bonds with other molecules of boron atoms. That's when the atoms are part of gamma boron, a whole new form of boron, the fifth element on the periodic table.



Courtesy of Artem R. Oganov

Using a special computer algorithm called USPEX, Oganov and his team were able to predict the crystal structure of a whole new form of boron — gamma boron (γ-B_{28}).

And it may be news for the rest of us, too. The study's ten-person research team made their discovery by using a special computer algorithm called USPEX. According to the study's lead researcher, Artem Oganov, USPEX has a bright future. "With our method," Oganov told *Today's Science*, "new materials can be found purely on the computer, and in rather short time. We believe it is the future of materials design."

The Good Old Days of X-Ray Crystallography

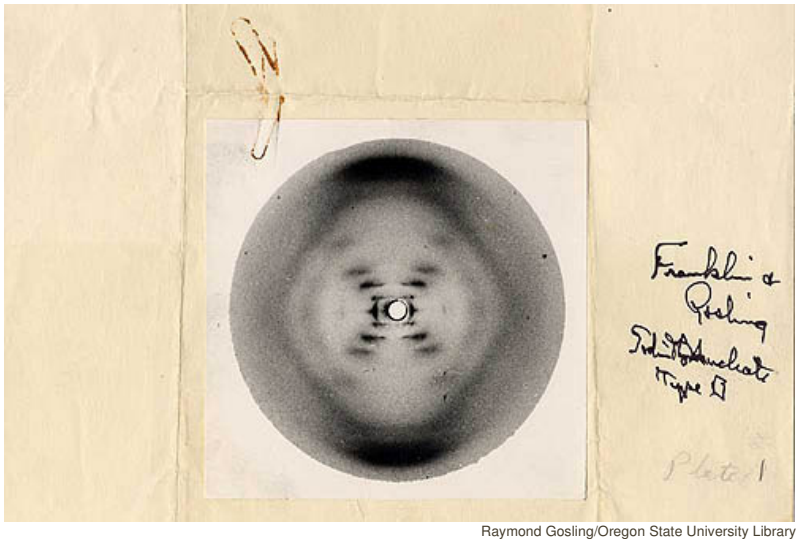
Several years back, Oganov teamed up with a computer whiz and another colleague to design a special

Structure of Atoms

Evidence, Models, and Explanation

computer program that predicts the structure of solid crystal materials. Using only a "chemical formula and fundamental laws of quantum mechanics," Oganov explained, his USPEX computer algorithm can predict crystal structures.

Normally, to figure out a molecule's crystal structure, scientists use an old method called X-ray crystallography. The most famous X-ray crystallographer to date is probably Rosalind Franklin, whose work on DNA allowed James Watson and Francis Crick to come up with their double helix model of the molecule. [See Talk and Toys Helped Watson and Crick Discover the Double Helix, May 1993]. Today, researchers continue to use X-ray crystallography to help them understand the geometry of many important molecules.



Raymond Gosling/Oregon State University Library

Franklin's X-ray crystallography of the B form, labeled Photograph 51. It was this photo that convinced Watson that the double helix was the key to the structure of DNA.

In brief, here's how X-ray crystallography works: researchers shine high-energy X-ray light at the molecule they want to study. When the X-rays hit the molecule, they bounce off in a particular way. If the sample molecule has a repetitive structure, as all crystals do, the X-rays will bounce off it in a special pattern that contains information about the crystal's structure. [See Scientists Illuminate Key HIV Protein Structure, August 1998; X-Ray Crystallography Reveals Cell Zipper, October 1995; Structure of Crucial Protein Revealed, October 1995].

In fact, the X-ray pattern looks nothing like the actual crystal. Crystallographers use math, inference, and their own trained eyes to transform the diffraction pattern into an actual picture of the crystal they're studying.

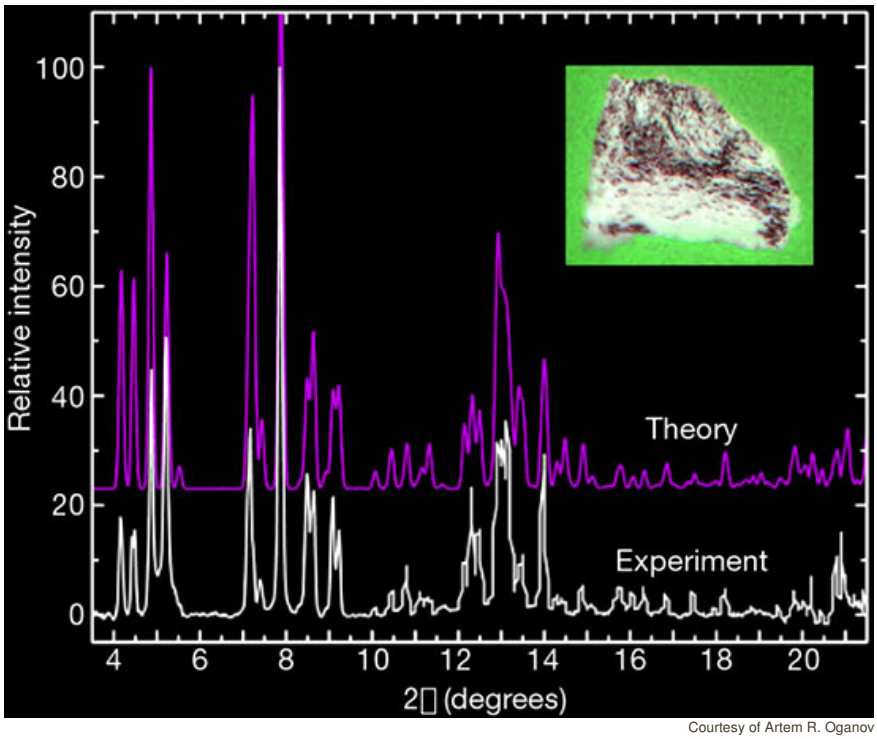
But Oganov and colleagues weren't satisfied with X-ray crystallography. At high temperatures and pressures, the method simply doesn't work well. X-ray crystallography is also a nuisance if you're trying to custom-make a molecule for a particular purpose. Imagine how much work would go into creating a molecule, testing whether it suits your needs, figuring out its crystal structure, and deciding how to tweak and improve your molecule. After perhaps years of research, you'd have to repeat these steps again and again to create a dream molecule.

Oganov says that his group's USPEX program "circumvents this difficulty and locates the most stable structure in a small number of steps."

USPEX Delivers

What USPEX stands for is rather pompous-sounding: Universal Structure Predictor: Evolutionary Xtrallography. But in fact, it's already helping researchers discover exciting new molecules.

USPEX is an example of what's called an evolutionary algorithm; its inner workings are inspired by evolution in biology. But it's simpler than that. In fact, we humans use evolution-like algorithms all the time, whether we're trying on bathing suits, learning how long to brew tea, or steering a car for the first time. One feature that unites all these activities, and biological evolution too, is that it's obvious when something works well. If you turn the steering wheel the right amount, you don't hit a tree. If you try on the perfect bikini, you rush to the beach. Likewise, when random genetic mutations somehow cause an animal to run faster and escape predators, the animal survives.



Courtesy of Artem R. Oganov

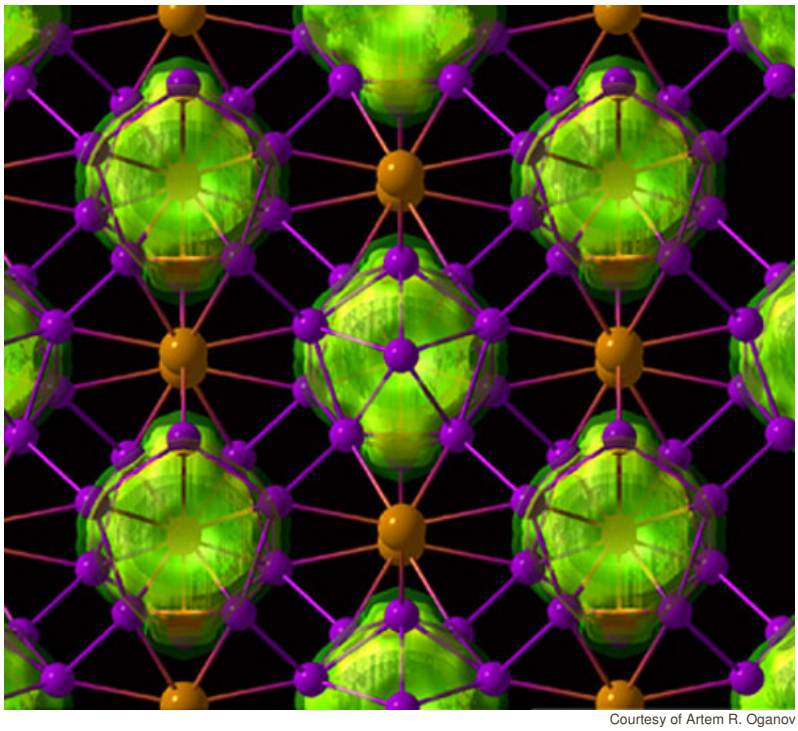
A graph comparing USPEX's energetic stability prediction for a configuration of boron atoms with Oganov's energetic stability experiment on the same configuration of boron atoms. He told *Today's Science* that "we made a number of bold predictions — and all of them have been confirmed by subsequent experiments."

But that doesn't mean it's easy to figure out how to pick out the right bathing suit or how long to brew a pot of tea. If you've never worn a bathing suit, you have no clue which style will be most flattering. If you've never made tea, you won't know the ideal brewing time. Instead, you basically start guesswork and then evaluate the results. Is your tea too bitter? Does zebra-print overemphasize your tummy? Based on the results of random trials, you make slightly smarter choices: say, brewing the tea less than five minutes, or trying on non-patterned bathing suits. This time, your tea comes out too weak, and the bathing suit is the wrong color for your skin tone. Such testing may take a long time, but eventually you find the perfect fit.

That's the idea behind evolutionary algorithms. They take a hard problem, make some random guesses, and learn from the results. The next time, the algorithms make slightly better random guesses, and see what happens. After enough repetition, you get brewed-to-perfection tea, and if you're using USPEX, you get stable and surprising molecular structures. The new form of boron is one such structure.

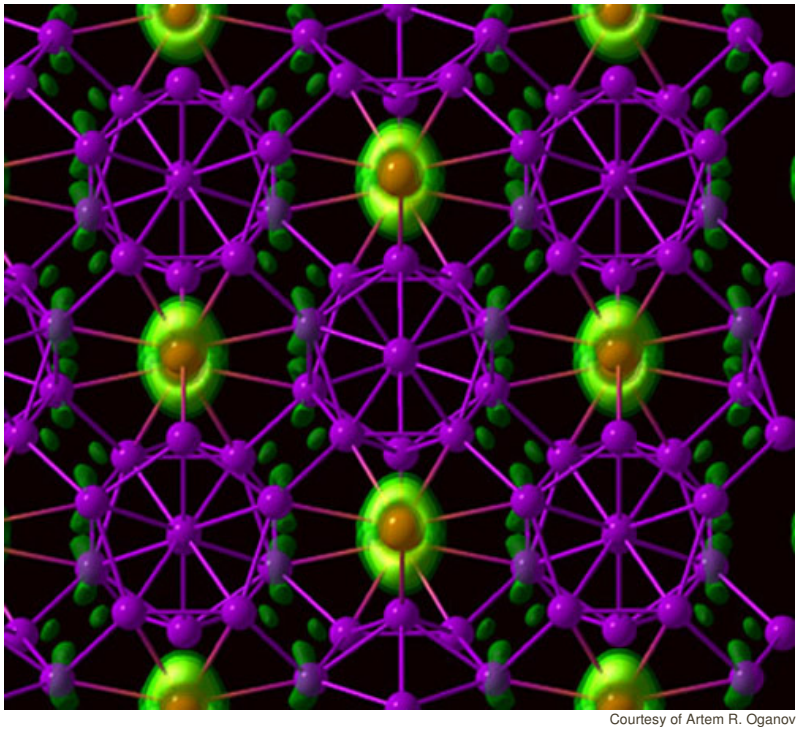
Gamma Boron: A Funky Form

Oganov's team set USPEX loose on boron to figure out what happens at high pressures. USPEX tested out the energetic stability of different configurations of boron atoms under different conditions, pruned away the unstable configurations, and hit upon a structure Oganov and colleagues named gamma-boron (γ-B_{28}, where the 28 corresponds to the number of boron atoms packed into the smallest non-repetitive chunk of the material).



Courtesy of Artem R. Oganov

Oganov and his colleagues pruned away the unstable configurations and came up with gamma-boron (γ-B_{28}). Panel A (above) shows the density of distribution of lowest-energy valence electrons; they are clearly concentrated on the B_{12} icosahedras. Panel B (below) shows the density of the lowest-energy unoccupied electronic states. These are concentrated on the B_2 pairs, indicating that B_2 pairs lose electrons and become positively charged.



Courtesy of Artem R. Oganov

In fact, researchers Jihad Chen and Vladimir Smoothen had synthesized this material back in 2004. But without help from USPEX, they couldn't figure out what they'd made. For the new study, Chen and Smoothen worked with Oganov and others to synthesize γ-B_{28} one more time. The team started with a very pure sample of a different form of boron, β-B_{106}, cranked up the temperature and pressure on their starting materials, and examined what came out. Using a method called X-ray electron probe microanalysis, they verified the purity of their final material. Also, to the extent that the group was able to analyze X-ray crystallography data of the

synthesized stuff—the samples were too small for complete analysis—they found a close match between USPEX's prediction and the real deal.

One neat feature of γ-B_{28} structure is that it's actually a two-for-one, made up of two substructures, B_{12} and B_2, each repeated twice to make B_{28}. These two substructures together form an ionic bond, where B_2 acts as an electron donor and B_{12} an electron acceptor. But the bonds between the two B_2 atoms and between the dozen B_{12} are of the covalent variety.

On periodic tables, boron appears on the boundary between metals and nonmetals; it's a metalloid with a dual nature. Boron also leads what chemists call the "*p* block" — the whole set of elements on the table's right-hand side. But despite its prominent position, boron is less famous than its two neighbors, aluminum and carbon.

Now, thanks to an evolutionary algorithm, we're learning more about boron's unique properties, its ability to bond iconically and covalently to itself, and its funky structure at high pressures.

What's more, we're learning about this structure through a method that's quick, easy, and as Oganov put it, "purely computational." If USPEX is as powerful as Oganov says it is, we'll be hearing more from this algorithm in the future.

Artem R. Oganov: Looking for Evolutionary Algorithms

Artem R. Oganov is currently an associate professor in the department of geosciences at the State University of New York at Stony Brook. He graduated from Moscow State University in 1997 and received his Ph.D. in crystallography from University College London in 2002. After post-doctoral research in Zurich, Switzerland, he joined the Stony Brook faculty in 2008.

Oganov's considers his major scientific focus "materials chemistry." His research involves "theoretical and computational physics, development of simulation methodologies and their application to studies of minerals at high pressures and temperatures, and to the design of new materials."

Below are Oganov's February 9, 2009 responses to questions posed to him by Today's Science.

Courtesy of Artem R. Oganov

"Modern science is based on experiment — as a theoretician I must admit this. Whether or not a prediction is correct is determined by its agreement with experiment."

Q. When did you realize you wanted to become a scientist?

A. At the age of 6. And I knew I would be a chemist.

Q. How did you choose your field?

A. I decided to become a chemist when I discovered in our Moscow apartment a popular book on chemical elements for kids. The book represented each element by a human-like picture and told exciting stories about the character and history of each element. I immediately fell in love with chemistry. My dream was to discover new chemical elements.

When I was 7 years old, my mother took me to evening lectures on chemistry. Students who attended those lectures treated me very well and called me "professor". The lectures were a bit too fast for me to write them down, so my mother took the notes. I treasure them till this day.

Then, at the age of 11, I started collecting minerals. With time, I decided to study the chemistry of Earth's and planetary materials. Quite early on I decided to do theory. This brought me to the development of theory of materials at high pressures and temperatures — those that reign in planetary interiors. This field is one of the fastest developing fields of chemistry and physics, with many exciting discoveries, including our discovery of the new form of boron. Such studies rely heavily on theory and computational techniques. Many important problems cannot be solved with today's computational methods — which prompted me to concentrate also on developing new computer simulation methodologies that would enable chemists to improve their understanding of matter. This addition of new research topics constantly widens my research area.

Q. Are there particular scientists, whether you know them in person or not, that you find inspiring?

A. I was always inspired by such people as Lev Landau, Michael Faraday, Linus Pauling, Gregor Mendel, Nicholas Steno, James Clerk Maxwell. I could tell many stories about each of them (and I do so in my classes), but the common traits of all these people are their passion, their charisma.

Among the big scientists whom I know personally, I have been most impressed with Michele Parrinello, Roald Hoffmann, Jack Dunitz, Karl Syassen.

Parrinello always impressed me with a great combination of creativity and rigor. Hoffmann, a Nobel Laureate, is a poet or an artist in science, he even writes plays and poems. His unique and sad life experience (he grew up in a concentration camp during WWII) and extremely warm personality (just like Jack Dunitz's) left a big impression on me. Karl Syassen, a high-pressure physicist, has impressed me with his deep love for science and encyclopedic knowledge. One of the very best experts in our field, he never advertised himself and maintained a remarkable lever of integrity and love for science.

Q. When you tell people you are do research in materials chemistry what is their reaction? What do you think is the biggest misconception about your profession?

A. My field is what I call "materials chemistry", "physical chemistry", "condensed matter physics" or "crystallography". The greatest misconceptions that people have is with the word "crystallography" - some think it's about religion, some that it's about occult healing with crystals, some that it's an old-fashioned science about shapes of crystals. The truth is that crystallography is a cutting-edge scientific discipline that explains and predicts properties of materials based on their structure. This includes all types of materials, inorganic or organic — even such as drugs, DNA, proteins. The number of Nobel prizes given to crystallographers is very large, it's several dozen. This science is at the very forefront of modern knowledge.

Q. Your latest study has been called "a beautiful example of cooperation between theory and experiment." Could you explain in simple terms to our student audience why your colleague Artem Bergara said this and what are the implications for future research?

A. Modern science is based on experiment — as a theoretician I must admit this. Whether or not a prediction is correct is determined by its agreement with experiment. In our study, we made a number of bold predictions — and all of them have been confirmed by subsequent experiments. This is why Prof. Bergara called our work a beautiful example of a cooperation between theory and experiment. In addition, our predictions were made using a new method developed by me and my research group. This work and the success of our predictions prove the power of our method.

Q. Where do you spend most of your workday? Who are the people you work with?

A. For me science is my life, I think about it even when I sleep or play with my daughter. It is a way of life. Most of my workday is spent at the university. I have a very unusual office — there is a bed, where I read literature and rest after lunch, and a small gym, which helps me to keep toned and remain in good shape. Apart from the office, I also have my own lab — it's a theoretical lab, so our main equipment is computers, libraries and computer visualization equipment. I also put beds and sports equipment in the lab, for people working there. People who work with me in the lab — I have a few grad students and one postdoctoral researcher, whom I moved to the U.S. from my previous work in Switzerland in December 2008. Soon I will hire a few more people. Apart from my own research group, I have very strong collaborations with several outside colleagues — in China, Germany, France, Italy and the U.S.

Q. What do you find most rewarding about your job? What do you find most challenging about your job?

A. What I like most is the constant learning about the way our world works — in my case, how the atoms determine the way materials work. I also like the element of a sport in my job — you must constantly overcome your own limitations, and when you discover something new, it's like climbing a high mountain. A unique feeling. A constant challenge to yourself.

Q. What has been the most exciting development in your field in the last 20 years? What do you think will be the most exciting development in your field in the next 20 years?

A. This is a hard question, there were several major developments. One was made in 1985 by [Roberto] Car and Parrinello, who invented a method enabling quantum-mechanical simulations of real-time dynamical evolution of atoms in materials. Another came from my own research in 2006 — it's a method, developed by me and my group, for predicting the most stable arrangements of atoms in a crystal. Mathematically, the problem is extremely complex, but we overcame it armed with ideas of Darwinian evolution. With this method we can design new materials with particular properties purely on the computer. Another major development, largely due to Karl Syassen's work, was the discovery that many simple elements display complex and counterintuitive behavior under pressure. Many examples were found for metals. Our work on boron, unexpectedly, extended this trend to non-metallic elements and uncovered new phenomena.

Q. How does the research in your field affect our daily lives?

A. Greatly. Just imagine where we would have been, had we not known the structure of matter? We would not be able to understand or improve materials around us, we would also not understand the way life and genetics work. We would know little of chemistry and physics, for many of their fundamental laws were discovered in my field. And now there is a great hope that we will soon be able to develop new materials completely on the computer.

Q. For young people interested in pursuing a career in science, what are some helpful things to do in school? What are some helpful things to do outside of school?

A. At school you should get the skills to learn, obtain maximum knowledge in scientific disciplines, and I would also add that you should pay attention to literature and history. Scientists have to express their ideas clearly and inspire the reader; each scientist is automatically also a writer. And history gives us priceless lessons, which should not be ignored. Another very important thing at school is to make friends. Outside of school, one should keep learning and developing oneself intellectually, mentally and physically.

Q. Just for fun: If you won the Nobel Prize, what would you do with the prize money?

A. I still have a lot of time to decide on this. I would spend a big part of that money to establish a small top-level research institute within my university, and a scholarship to help the best students.

Discussion Questions

Do you think evolution type algorithms will always yield the best possible result? Suppose you are lost on top of a mountain and your aim is to get down to the road as fast as possible; will picking your direction based on what is the steepest downhill-grade always work? Look up "greedy algorithm" and see how that compares to the sort of algorithm described in this article.

Journal Abstracts and Articles

(Researchers' own descriptions of their work, summary or full-text, on scientific journal websites).

"Ionic High-Pressure Form of Elemental Boron." www.nature.com/ nature/ journal/ v457/ n7231/ abs/ nature07736.html.

"USPEX—Evolutionary Crystal Structure Prediction." www.bionik.tu- berlin.de/ user/ niko/ CPC- USPEX- 2006.pdf.

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"Electron Probe Technique and Instrumentation," Informational website hosted by John Donovan of the Chemistry Department, University of Oregon. (August 5, 2006) [accessed Feb. 12, 2009]: epmalab.uoregon.edu/ epmatext.htm.

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Keywords

boron, boron crystal structure, X-ray crystallography, evolutionary algorithms, USPEX, Universal Structure Predictor: Evolutionary Xtrallography, Artem R. Oganov

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