On the Trail of **Tomorrow's Semiconductors**

In the quest for new semiconductors, researchers are no longer relying on experiments alone. In an approach that could be a game changer for photovoltaics and computing applications, physicist Harald Oberhofer and his team are developing computer models capable of analyzing just about every conceivable material.

Harald Oberhofer's group at the Chair of Theoretical Chemistry

www.th4.ch.tum.de/oberhofer/

Reinhard Kleindl

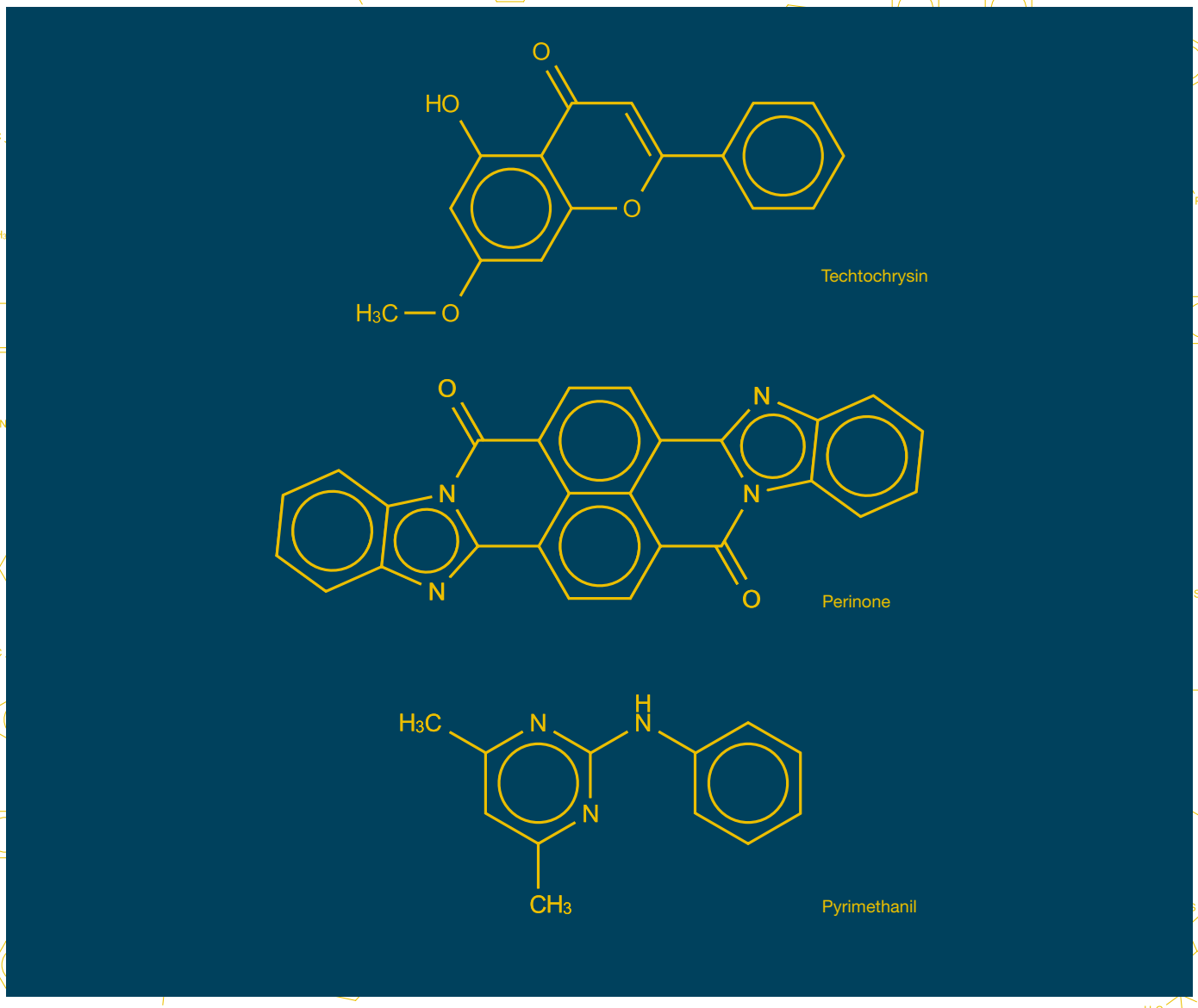
Wo steckt der Halbleiter von morgen?

Mehr als 10.000 Materialien aus unterschiedlichen Einsatzbereichen wie etwa der Pharmakologie haben Wissenschaftler um Dr. Harald Oberhofer auf ihre Halbleiter-Eigenschaften hin untersucht. In Laborversuchen wäre das nicht durchführbar. Möglich wird es mithilfe ausgefeilter Computermodelle und riesiger Datenbanken, in denen die Eigenschaften hunderttausender Materialien gesammelt sind. Oberhofer ist Leiter einer Forschungsgruppe am Lehrstuhl für Theoretische Chemie der TUM – und das, obwohl er eigentlich Physiker ist. Das ist kein Zufall, auch die Chemie basiert auf physikalischen Vorgängen. Der 37-Jährige sucht mit seinen Computermodellen nach neuen Halbleitern, die nicht auf Silizium basieren, sondern auf Materialien der organischen Chemie, also Kohlenstoffverbindungen.

Einige dieser organischen Halbleiter haben längst ihren fixen Platz in der Technik, etwa organische Leuchtdioden, bekannt als OLED. Organische Solarzellen hingegen, die eine besonders kostengünstige Stromversorgung versprechen, kranken nach wie vor an der schlechten Haltbarkeit im Sonnenlicht. Dass es geeignetere Materialien gibt, ist nicht auszuschließen, die meisten organischen Halbleiter sind nach wie vor unerforscht.

Die Menge der theoretisch möglichen organischen Verbindungen ist zudem gigantisch. Oberhofer konnte unter den 10.000 untersuchten Materialien eine Handvoll organischer Stoffe identifizieren, die über eine ausreichende Leitfähigkeit verfügen, um als Halbleiter geeignet zu sein. Diese können nun einer genaueren Analyse unterzogen werden. Dann wird sich zeigen, ob sich darunter Materialien für beständigere Solarzellen finden. □

Graphics: ediundsepp (source: TUM)



Using theoretical screening methods, Harald Oberhofer's team has identified several molecules with good semiconductor properties. These include:
// Techtochrysin, a flavonoid present in sour cherry
// Perinone, a red pigment that is already used as a semiconductor
// Pyrimethanil, a fungicide used in herbicides

"With the help of computer simulations we can obtain very detailed insights – into the structure of 10,000 different molecules."

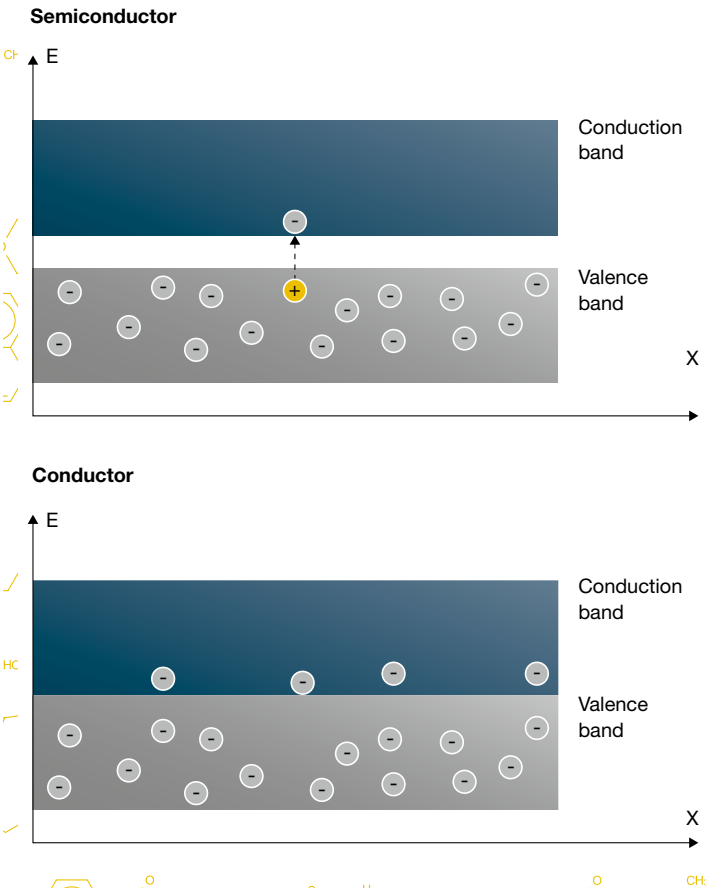
Harald Oberhofer

Breakthroughs in the history of technology have often been sparked by the discovery of new materials and exploration of their properties. New knowledge about semiconductors paved the way for the Information Age, just as the ability to produce bronze by smelting copper and other alloys marked an end to the Stone Age. In many cases, the discovery of new materials and their specific properties was simply a matter of luck.

Nowadays, the understanding of matter at a chemical level is so extensive that certain research groups are no longer willing to rely on chance. They have started to theoretically determine the properties of thousands of materials in the search for highly specific capabilities that would be promising for various technical applications. This process is known as "theoretical screening". One researcher involved in this field is physicist Dr. Harald Oberhofer from TUM. His mission is to find the semiconductors of the future and open up new opportunities in photovoltaics or the manufacture of energy-efficient electronics.

Virtual microscope

"This is the best microscope in the world," says Harald Oberhofer with a knowing smile. He works as a research group leader at TUM's Chair of Theoretical Chemistry on the Garching Campus. Sitting in his office, he looks at a screen as he writes lines of code in the Python and Fortran programming languages. The programs he is creating along with his research group will soon be running on one of Europe's fastest supercomputers. The SuperMUC is only a few buildings away at the Leibniz Supercomputing Center. Acting like a virtual microscope, it will provide in-depth insights into the electrical behavior of an extremely large number of chemical compounds. ▷

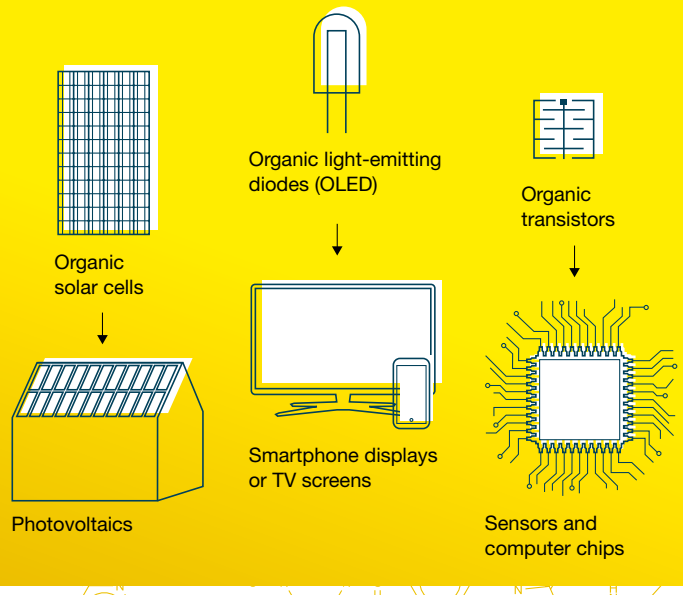


The difference between conductors and semiconductors lies in the way the electrons behave. Whereas conductor electrons (bottom) are highly mobile and begin to flow with the slightest external charge, electrons in semiconductors (top) need to reach a certain threshold energy before they can flow freely – illustrated by the gap in the middle of the image; also known as the "band gap". Absorbed light can energize the electrons to the required level, an effect that is used in photovoltaics.

Semiconductors

Semiconductors are materials that conduct electricity under certain circumstances. The best-known example is the element silicon. Somewhere between insulators, which hardly conduct any electricity at all, and conductors, which have excellent conductive properties, semiconductors offer differing degrees of efficiency depending on various factors. One of these is temperature. At low temperatures, semiconductors do not conduct electricity whereas they do when the temperature rises to a certain point. The opposite is the case with conductors such as metals, for instance, where conductivity generally drops as the temperature rises. It is possible to selectively modify the electronic properties of a semiconductor material by doping it (i.e. by introducing foreign atoms). Semiconductors can be used to fabricate diodes, transistors and even computer chips – hence the reference to the "semiconductor industry".

Usage of organic semiconductors



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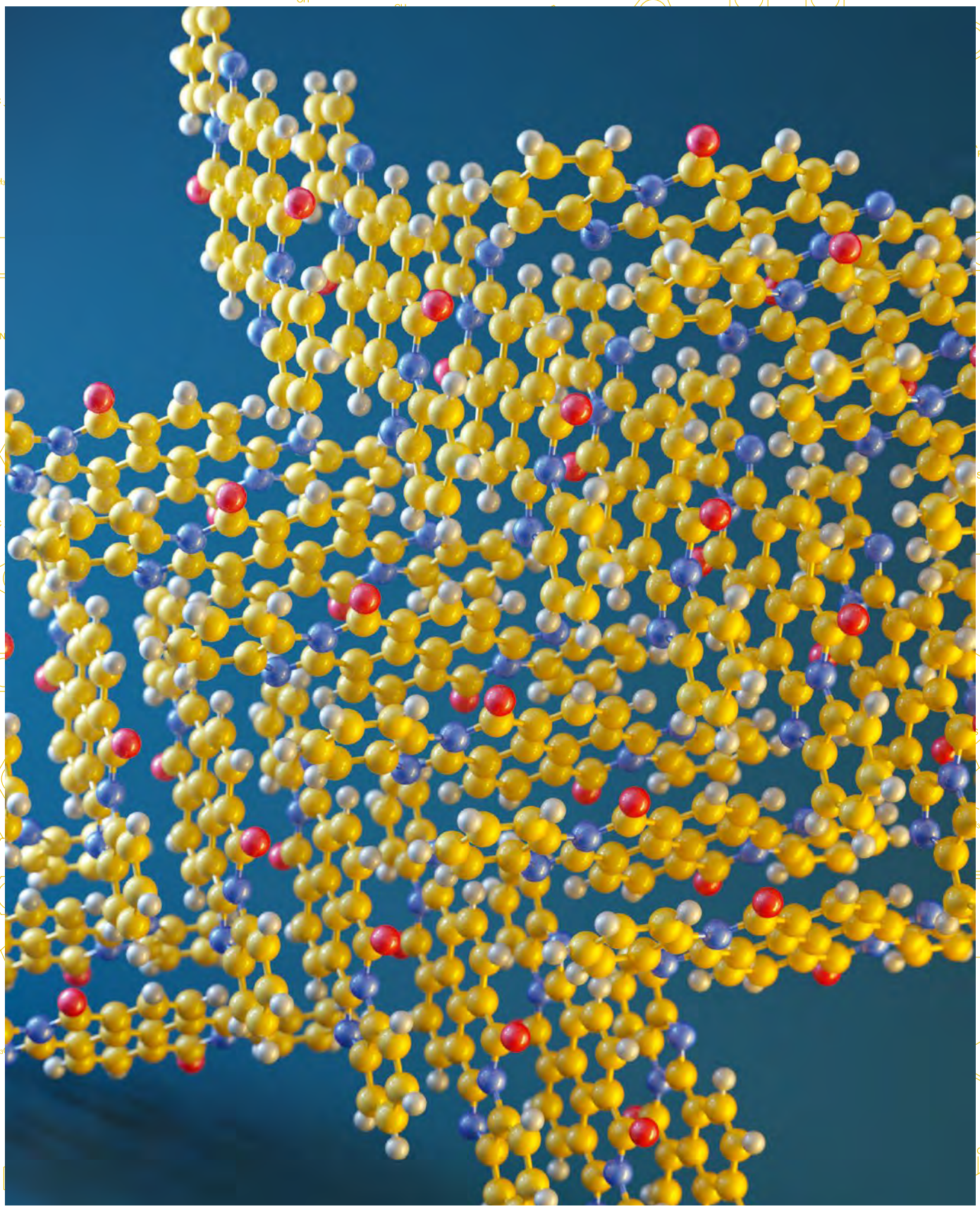


In solid form, organic molecules can be organized into a structure known as a crystal. The scheme shows a crystal of perinone, a red pigment with semiconductor properties. The molecule is composed of oxygen (red), nitrogen (blue), carbon (yellow) and hydrogen (white).

Oberhofer is especially interested in organic materials, and wants to find out if they have potential as semiconductors. Here the word “organic” refers to the field of organic chemistry that deals with carbon compounds, including plastic in all its forms.

Organic semiconductors are already widely used by some manufacturers – smartphone screens being one good example. They work with what are known as OLEDs – organic light-emitting diodes.

Short-lived solar cells

The weakness of organic semiconductors lies mainly in their limited lifespan, in particular in the case of solar cells. The fact that they are continuously exposed to UV light means that they are subject to degradation to a certain extent. “Organic solar cells do have a lifespan problem,” admits Oberhofer. Which is why the researchers are keen to find materials that selectively convert the absorbed UV light without resulting in degradation. There is a good chance of success given that up to now, only a fraction of potential organic semiconductor materials have been investigated. This is what Oberhofer wants to change with his research. With the help of computer models, he calculates charge transfer in solids made of organic molecules. ▷

Theoretical screening

All modern natural science disciplines rely on theoretical research. Experiments are supplemented and supported by this type of research and, increasingly, computer simulations. Theoretical chemistry has two threads. On the one hand, research groups try to gain a detailed understanding of what happens within experiments and develop recommendations for improvements or new tests. On the other hand, independently of the experiment, they are on the quest for something completely new, such as identifying promising materials that were previously used in a completely different context. This process is known as “theoretical screening”. The line between theory and experiments is becoming somewhat blurred now that experimenting researchers are increasingly likely to carry out their own computer simulations.

Harald Oberhofer at the Leibniz Supercomputing Centre: His complex calculations run on the SuperMUC, one of Europe’s fastest supercomputers.

Graphics: edfundsepp (source: TUM); Picture credit: Kurt Bauer/TUM

"The big advantage of computer simulations is that we can obtain very detailed insights into the structure of molecules," describes Oberhofer. "We see where the electrons are located – something that is very hard to do in an experiment. We begin by looking at large international materials databases." These list all materials produced and characterized by various research groups over the decades, including everything from drugs to components of crude oil. "We use our computational models to screen for promising organic semiconductor candidates," says the 37-year-old physicist.

Sea of molecules

Oberhofer calls up a screen showing arrangements of colorful spheres representing molecules. "One of the things that determines whether a material has semiconductor potential is the ease with which individual electrons jump from one molecule to another," he explains. The greater the overlap between the electron orbitals, i.e. the higher the electron density, the more likely this is. Another criterion is the amount of energy an electron requires to make the switch from one molecule to another. When both effects are considered together, useful information can be gleaned about the material's conductivity.

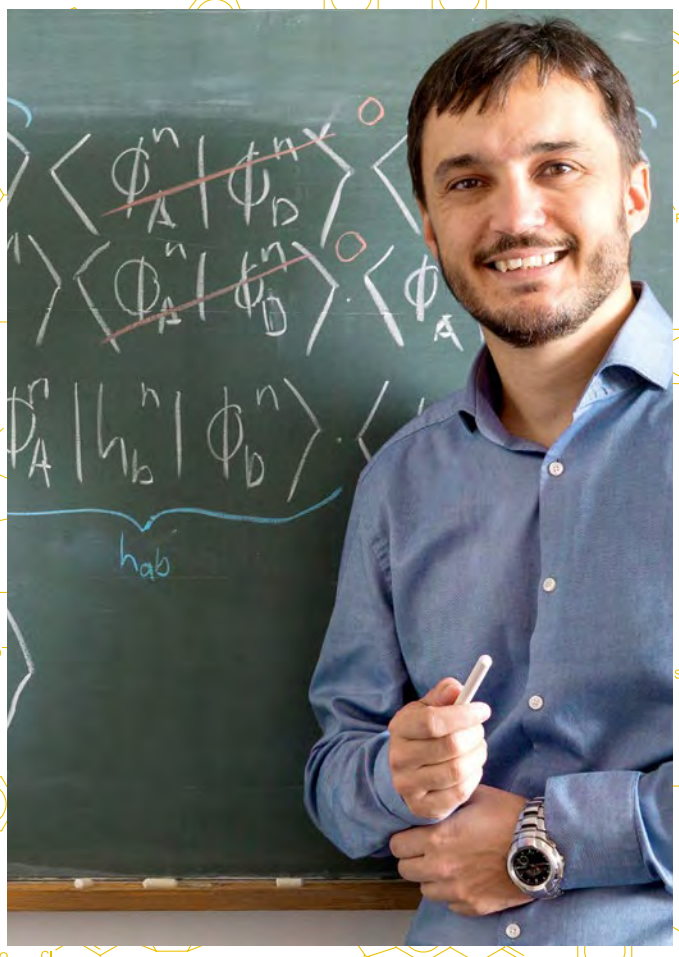
Oberhofer's analysis is based on what is known as the "density functional theory". This is a method from quantum physics which can be used to calculate the distribution of electrons in molecules.

According to Oberhofer, the only way to perform such analyses is by using theoretical methods: "The substances we are investigating can be costly and difficult to get a hold of. Some of them we even have to synthesize before we can obtain crystals and then run extensive tests," Oberhofer explains. "You can do that up to a certain point, but not for the 10,000 systems that we screened using our method. We only select the most promising candidates for more detailed investigation," says Oberhofer. Through this work, he produces valuable pointers for his colleagues' experiments. "The huge number of possible molecules gives us massive scope for semiconductor candidates," adds Oberhofer.

Interesting material discoveries

"We have managed to identify a few materials from completely different application scenarios that have good semiconductor properties. They include a pigment and a fungicide," says Oberhofer, who is now planning to investigate the most promising candidates using more precise theoretical methods. One of them could prove to be the ideal semiconductor for the solar cells of tomorrow.

Reinhard Kleindl



Dr. Harald Oberhofer

A theoretician at heart

Harald Oberhofer is head of a research group at TUM's Chair of Theoretical Chemistry (Prof. Karsten Reuter) even though he actually qualified as a physicist. That is not so unusual, however, since chemistry is also based on physical processes. "For me, the development of methodologies has always been my main interest. I really enjoy working away at intricate 'puzzles' like these," admits the 37-year-old scientist.

Originally from Vienna (Austria), he obtained his doctorate from the University of Vienna with a thesis on statistical mechanics. During three years of research at the University of Cambridge (UK), he developed an interest in the simulation of charge transfer. His current research is focused on the search for new organic semiconductors, photocatalysts and metal-organic frameworks.

Graphics: ediundsepp (source: TUM); Picture credit: Kurt Bauer/TUM