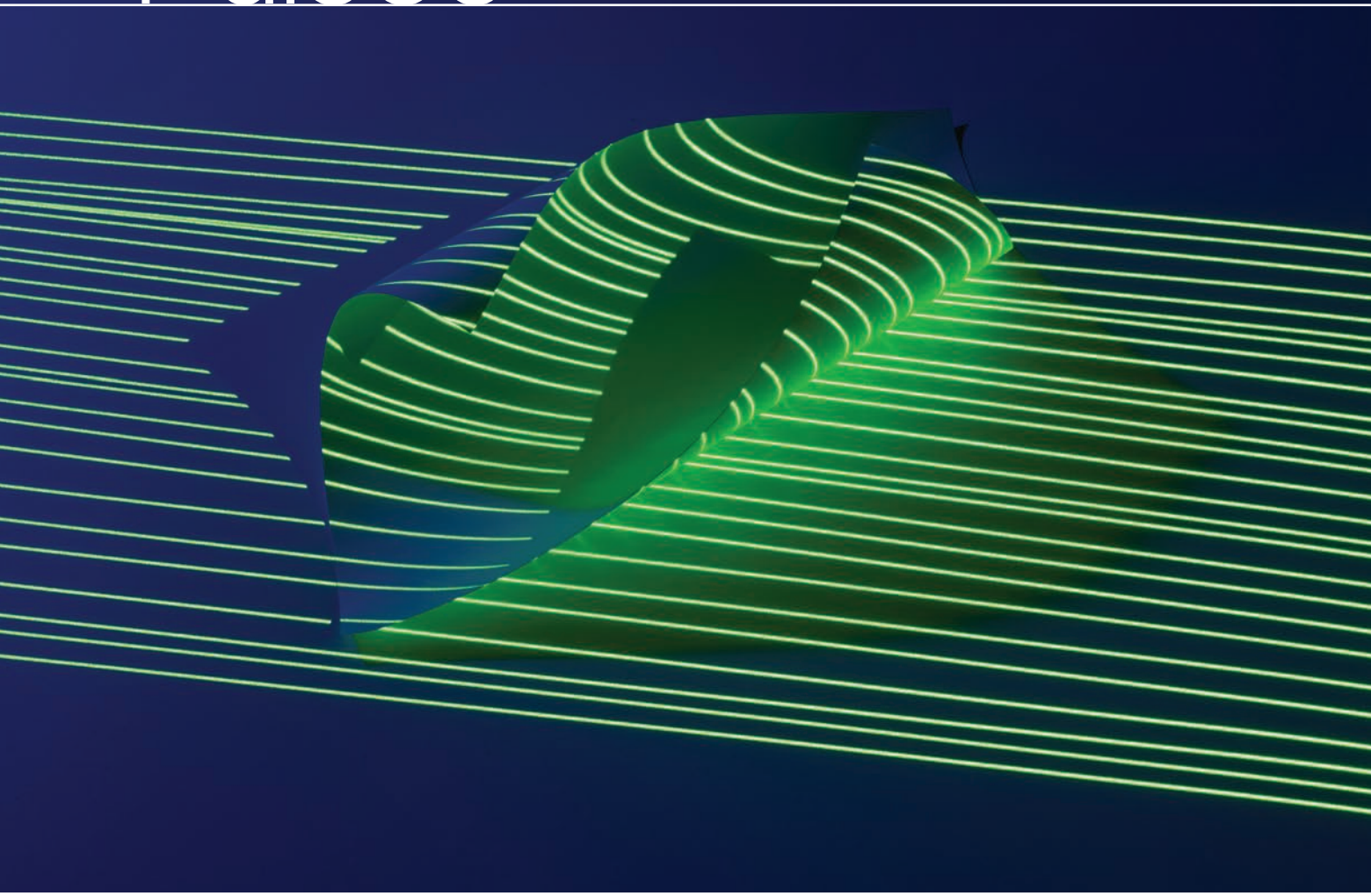

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CONVERSATIONS

Treasure Maps for Optical Materials

At the 2022 Advanced Photonics Congress, materials scientist **Matthias Wuttig** will talk about how mapping chemical bonds to material properties can offer shortcuts for designing novel optical materials.

The 2022 Advanced Photonics Congress, taking place from 24 to 28 July in Maastricht, Netherlands, as well as online, will highlight the latest advances in optical materials, optical signal processing, optical communications and integrated optics. OPN talked with one of the four plenary speakers of the congress, Matthias Wuttig, a materials scientist at RWTH Aachen University, Germany, who says he is very excited to be attending the event and talking with optics and photonics researchers about his research in optical materials.

Q. What's the biggest thing driving the optical-materials field today?

In modern society, photonic technology plays a very prominent role. But we would like to expand the application area of photonics. Currently, many of these photonic devices are static, which means that when a photon is redirected by the device, it's always redirected in the same direction. We would like to have a photonic switch where, under a certain condition, the light goes one way, and under another condition, the light goes another way.

This requires active materials, in which we can modify the optical properties. With most materials that we currently have, it's almost impossible to change their optical properties. But there are unconventional materials where a change in atomic arrangement leads to a significant change in optical properties.

And this is something that you can utilize for a number of applications. You can use this for displays, switches and so on. So there's a big hope that, with such active materials, you can realize novel photonic functionalities. This is the main driver of the field. And as a materials scientist, I would love to be able to design materials that meet the specific needs of the photonic industry. One example would be a mirror that can reflect the light, and then, let's say, when you apply an electrical voltage, it becomes transparent.

This is precisely what is exciting to materials scientists. And that's why I'm so happy to go to the Advanced Photonics Congress—to basically talk with people on the application side and ask, "Hey, what do you need?"

Q. What sort of things go into answering that question?

There are a couple of things we're trying to accomplish with optical materials. For example, the key property of a lens when focusing light is the refractive index. If you can alter the refractive index, you can do more with the same lens. And switching between the mirror and the transparent material—the example that I mentioned earlier—is basically achieved by changing the plasmonic material response. And if you can turn on or off this mirror property of material, this gives you another area for a cool application.

There's already some divergence in the field. Some people are interested in changing the refractive index; others are interested in the plasmonic material response or the absorption of the material. But if we think further, it's not only about how strongly you can change optical properties. It's also about how fast you can switch. Another important element is power consumption. How much power do I need to switch material back and forth? Reliability is important, too.

So there's a whole set of important design parameters. And, for us, as materials scientists, it's crucial to speak with people on the application side to hear their wish list. Although if they want a material with a huge change in refractive index that works in a picosecond with minimal power consumption, we might have to say that such a material has not been found yet, and we're not even sure if we can ever find it.

Courtesy of M. Wuttig

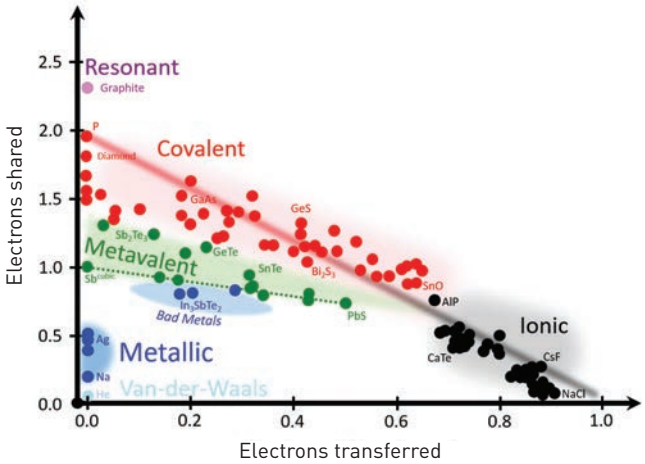
> "If we have a map that describes trends in chemical bonding, this map should tell us where we would find certain properties, because chemical bonding and properties are related."
>
> *—Matthias Wuttig, RWTH Aachen University, Germany*

Q. What are the "treasure maps" that your team has developed for these design problems?

We're trying to find a novel way of designing materials. There's a close relationship between chemical bonding and [physical] properties. So, if we have a map that describes trends in chemical bonding, this map should tell us where we would find certain properties, because chemical bonding and properties are related.

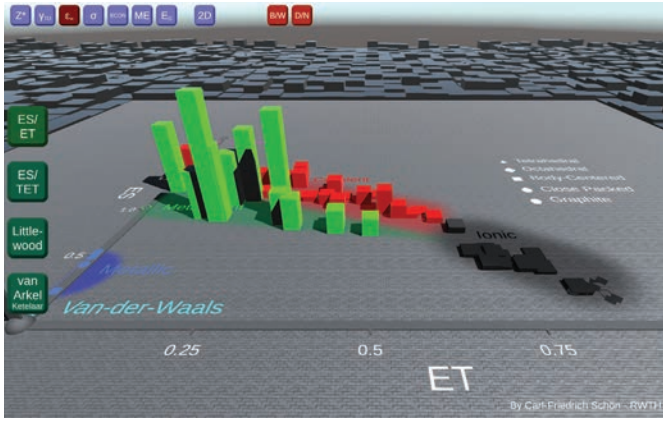
We have learned in chemistry classes about covalent bonding, ionic bonding, metallic bonding, Van der Waals bonding and hydrogen bonding. But when you try to imagine a transition from covalent to metallic, for example, the language we use to describe each bonding is so different, you don't have the language to describe the transition. So, we said "We need one language." Then, we built a map using quantum chemical bonding descriptors that are excellent property predictors.

So now, if a company comes to us and tells us which properties



2D map classifying chemical bonding in solids.

L. Guarneri et al. Adv. Mater. **33**, 2102356 (2021), CC BY-NC 4.0



3D, interactive map classifying chemical bonding in solids.

C.-F. Schön, materials-map.rwth-aachen.de

they need in their material, we can look at the map and find relevant materials. The key goal is to provide a map that describes systematic trends in chemical bonding, which translate into systematic trends into material properties.

Q. What does such a map actually look like?

It has two different coordinates—we look at charge transfer between atoms and the sharing of electron pairs between atoms. It turns out that there's an area of metavalent bonding, which we color green on our maps, where many of these interesting materials are that you can use as active photonics switches. In the green region, there are many chalcogenides—these compounds of sulfur, selenium and tellurium. They have these special properties. And now we have to check which other materials might also have the same properties.

We have also developed an interactive, 3D map that lets you look at a typical property. When you click on a certain optical property—for example, the one linked to refractive index—the map would show materials' refractive indexes in a bar graph. This map is publicly available, but I do believe we can provide some important insights in guiding people how to use this map, since in the very end, the true map that you would need to look at is not three-dimensional; it's maybe seven- or eight-dimensional.

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> *—Matthias Wuttig, RWTH Aachen University, Germany*

Q. Seven or eight dimensions—that sounds complicated.

Yes—you have to have basically think in a multidimensional property space. Finding your way around in that kind of property space needs either experience, a deep understanding or very sophisticated computer algorithms, to basically tell you how you can balance all of the different requirements for materials that you have. We are also building up a much, much larger database, soon extending this to a thousand materials.

Q. Where do you think applications of optical materials are headed?

Optical materials are for more than just communication. You can also use these materials for displays. You can use them for routers. You can use them for metamaterials.

So I really hope that this plenary talk [at the Advanced Photonics Congress] will inspire the photonics community to dream big. What could you do if you had a material which can have such a fantastic change of optical properties? And which kind of applications can you envision? I am really hoping to learn from the needs and dreams of the photonic-application industry. OPN