Department of Physics & Astronomy
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Catching Rays

UT physicists look at turning sunlight into current

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Energy, it turns out, can be free, but only if you know how to catch it. That's the hope for photovoltaics, which take solar radiation and convert it to electric current. But getting to that point requires a deeper understanding of the physics behind this process, and UT's condensed matter physics group has been working with titanium dioxide (TiO_2) to investigate that potential. In collaboration with Physics Professor Hanno Weitering, Associate Professor Norman Mannella's research group described this research in *Physical Review Letters* in late January.

"TiO_2 is an important system to study because there is an abundance of titanium in the Earth's crust," Mannella said. "It is incredibly robust," making it a good candidate as a catalyst to stimulate photoreactions.

Solid materials have a structure made up of energy bands. Materials such as TiO_2 have a valence band, occupied by electrons, and an empty band above it referred to as the conduction band. The energy difference between them is called the band gap. Unfortunately, TiO_2 also has a major drawback. In TiO_2, the band gap is too wide to absorb the full spectrum of sunlight: it can only absorb the ultraviolet.

"The band gap of TiO_2 is, unfortunately, about three electron volts, so a big portion of the spectrum from the sun is not absorbed by TiO_2 because it passes through," Mannella explained. "So if we want to exploit the energy coming from the sun that is free, we want to shrink the band gap so that more of the light is absorbed."

But "shrinking the band gap is not the whole story," he continued. "It's something which is necessary, but not sufficient to achieve your goal: the goal being that you want to have, say, a photoconductive material."

While narrowing the band gap means absorbing more light, this is not very helpful if you can't convert it into an electric current, and that requires movement.

"Energy (from the sun) is able to take some electrons that are sitting in the valence band and put them in the conduction band because now you have shrunk the band gap," Mannella said. "But if these electrons that you have put in the conduction band and, consequently, the holes that you have formed in the valence band do not move, you are stuck. Remember that your goal is to generate the current. Ideally, you would like electrons and holes to be able to move, otherwise you won't have current.

"Unfortunately, nature fights you back," he continued, "because absorption of light puts an electron in the conduction band, and a hole, positively charged, in the valence band, and they tend to recombine. This is known as the exciton recombination. You need to produce current. If the charge(s) that you create combine very fast, you are dead in the water."

To work around this problem, former UT Physics faculty member Zhenyu Zhang looked at ways to change the structure of titanium dioxide by enhancing the doping scheme, a method that adds electrons or holes. Typically a doping approach involves adding two elements donating charge in equal amounts: three electrons and three holes, for example. This is called "compensated" doping. Zhang and his colleagues went a different route with non-compensated co-doping.

The approach can be compared to altering a recipe, such as tweaking how you'd bake a cake by adding chocolate chips. Mannella said what is remarkable here is that by adding only 2-to-3 percent of doping atoms such as chromium and nitrogen, the properties of TiO_2 can change drastically.

“It is like putting very few chocolate chips in a cake, and the latter tastes completely different!” he said.

By co-doping TiO_2 with chromium and nitrogen atoms, researchers found that they could not only shrink the band gap by one electron volt, but also that their experiments indicated the electrons are not locked in position, but move away.

“Our work has demonstrated experimentally the validity of the non-compensated doping approach,” Mannella said. “In addition to demonstrating the shrinking of the band gap, our measurement(s) indicate that when electrons are excited in the conduction band, they tend to delocalize very fast. This is promising because it looks like you may be close to make an efficient device out of doped TiO_2.”

In the scientific sense, he said, this work addresses a general problem many condensed matter physicists encounter: “namely, the fact that it is really difficult to dope oxides.” But “in the broader context, it’s our belief that if you want to control the properties of matter, you need to understand it first.”

UT physicists Christine Cheney, Paolo Vilmercati, and Hanno Weitering are co-authors on the PRL paper, as are Mannella and emeritus professor Tom Callcott and UT bachelor’s graduate Eric Martin, now at the University of Colorado. Co-authors from collaborating institutions are Mirco Chiodi and Luca Gavioli of the Catholic University of the Sacred Heart in Brescia, Italy, as well as Murari Regmi and Gyula Eres of Oak Ridge National Laboratory.