Revealing the microscopic mechanisms in perovskite solar cells

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A material with the perovskite crystal structure has become very popular for solar cells. While most perovskites are inorganic compounds, this new material is a hybrid of relatively inexpensive organic and inorganic materials. In just a few short years, researchers have achieved remarkable power conversion efficiency with these perovskites, comparable with the best photovoltaic materials available.

Now, researchers from Japan have revealed the physics for how an important component of a perovskite solar cell works—a finding that could lead to improved solar cells or even newer and better materials. They describe their experiments in this week's issue of the journal *Applied Physics Letters*.

"The main studies have focused on improving [solar cell] efficiency [with perovskite]," said Kazuhiro Marumoto of the University of Tsukuba. "But the microscopic mechanism behind [how] these solar cells [using perovskites work] has not been fully investigated."

Solar cells work by converting light energy into electricity. When a photon strikes the perovskite, for example, it knocks an electron loose. The empty spot vacated by the electron is called a hole, and acts as a positively charged particle. The subsequent motion of the electrons and holes is what generates electrical current.

Because the perovskite itself doesn't conduct the movement of holes very well, solar cells require an additional layer of a hole-transport

material to facilitate current flow. One common hole-transport material is a compound called spiro-OMeTAD. To boost the current even more, researchers add a lithium salt called LiTFSI to spiro-OMeTAD. This process is called "doping."

Spiro-OMeTAD is an amorphous material, which gives it some unique properties. Most solid materials have well-defined electronic energy bands in which electrons and holes can move to transport through the material. Crystals, for example, often have band structures that allow for symmetric flow of both electrons and holes. But amorphous materials don't.

Due to this asymmetric band structure, holes can have a difficult time traveling through an amorphous material because they can get trapped in a particular energy level. But, according to theory, doping spiro-OMeTAD with LiTFSI prevents the holes from getting trapped.

Pairs of electrons occupy each energy level in spiro-OMeTAD. But when LiTFSI is introduced, one of those electrons is removed, leaving behind a hole in its place. The presence of that hole prevents other holes from getting stuck at that energy level, allowing them to move freely and generate electrical current.

Previously, no one has confirmed this process. But Marumoto and his colleagues have now used electron spin resonance (ESR) spectroscopy to show that this mechanism is, in fact, responsible for improving the ability of spiro-OMeTAD to carry current.

ESR spectroscopy measures the spin of single, unpaired electrons, which is what's created when spiro-OMeTAD is doped with LiTFSI. In experiments without light, the researchers found that the number of electron spins in spiro-OMeTAD increased by two orders of magnitude after being doped, confirming the effect of LiTFSI.

To see how doping affects the efficiency of a perovskite/spiro-OMeTAD solar cell, the researchers then conducted their experiments on the two materials layered together, with the lights on. The light induces holes to transfer from perovskite to spiro-OMeTAD and generate electric current. The researchers found that doping boosted this hole transfer, demonstrating how LiTFSI improves the efficiency of a solar cell.

More information: Miki Namatame et al, Direct observation of dramatically enhanced hole formation in a perovskite-solar-cell material spiro-OMeTAD by Li-TFSI doping, *Applied Physics Letters* (2017). DOI: 10.1063/1.4977789

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