Getting more electricity out of solar cells

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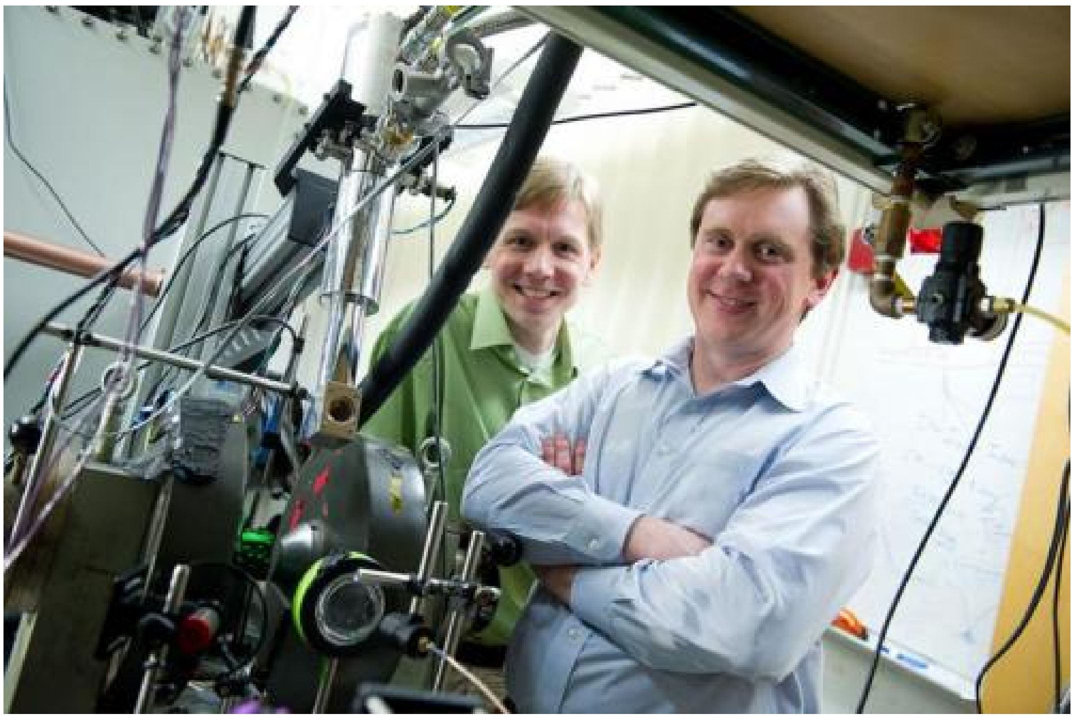

Troy Van Voorhis, professor of chemistry (left), and Marc Baldo, professor of electrical engineering (right). Credit: Stuart Darsch

(Phys.org) —When sunlight shines on today's solar cells, much of the incoming energy is given off as waste heat rather than electrical current. In a few materials, however, extra energy produces extra electrons—behavior that could significantly increase solar-cell efficiency.

An MIT team has now identified the mechanism by which that phenomenon happens, yielding new design guidelines for using those special materials to make high-efficiency solar cells. The results are reported in the journal *Nature Chemistry* by MIT alumni Shane R. Yost and Jiye Lee, and a dozen other co-authors, all led by MIT's Troy Van Voorhis, professor of chemistry, and Marc Baldo, professor of electrical engineering.

In most photovoltaic (PV) materials, a photon (a packet of sunlight) delivers energy that excites a molecule, causing it to release one electron. But when high-energy photons provide more than enough energy, the molecule still releases just one electron—plus waste heat.

A few organic molecules don't follow that rule. Instead, they generate more than one electron per high-energy photon. That phenomenon—known as singlet exciton fission—was first identified in the 1960s. However, achieving it in a functioning solar cell has proved difficult, and the exact mechanism involved has become the subject of intense controversy in the field.

For the past four years, Van Voorhis and Baldo have been pooling their theoretical and experimental expertise to investigate this problem. In 2013, they reported making the first solar cell that gives off extra electrons from high-energy visible light, which makes up almost half the sun's electromagnetic radiation at the Earth's surface. According to their estimates, applying their technology as an inexpensive coating on silicon solar cells could increase efficiency by as much as 25 percent.

While that's encouraging, understanding the mechanism at work would enable them and others to do even better. Exciton fission has now been observed in a variety of materials, all discovered—like the original ones—by chance. "We can't rationally design materials and devices that take advantage of exciton fission until we understand the fundamental mechanism at work—until we know what the electrons are actually doing," Van Voorhis says.

To support his theoretical study of electron behavior within PVs, Van Voorhis used experimental data gathered in samples specially synthesized by Baldo and Timothy Swager, MIT's John D. MacArthur Professor of Chemistry. The samples were made of four types of exciton fission molecules decorated with various sorts of "spinach"—bulky side groups of atoms that change the molecular spacing without altering the physics or chemistry. To detect fission rates—which are measured in femtoseconds (10-15 seconds)—the MIT team turned to experts including Moungi Bawendi, the Lester Wolfe Professor of Chemistry, and special equipment at Brookhaven National Laboratory and the Cavendish Laboratory at Cambridge University, under the direction of Richard Friend.

Van Voorhis' new first-principles formula successfully predicts the fission rate in materials with vastly different structures. In addition, it confirms once and for all that the mechanism is the "classic" one proposed in 1960s: When excess energy is available in these materials, an electron in an excited molecule swaps places with an electron in an unexcited molecule nearby. The excited electron brings some energy along and leaves some behind, so that both molecules give off electrons. The result: one photon in, two electrons out. "The simple theory proposed decades ago turns out to explain the behavior," Van Voorhis says. "The controversial, or 'exotic,' mechanisms proposed more recently aren't required to explain what's being observed here."

The results also provide practical guidelines for designing solar cells with these materials. They show that molecular packing is important in defining the rate of fission—but only to a point. When the molecules are very close together, the electrons move so quickly that the molecules giving and receiving them don't have time to adjust. Indeed, a far more important factor is choosing a material that has the right inherent energy levels.

The researchers are pleased with the agreement between their experimental and theoretical data—especially given the systems being modeled. Each molecule has about 50 atoms, and each atom has six to 10 electrons. "These are complicated systems to calculate," Van Voorhis says. "That's the reason that 50 years ago they couldn't compute these things—but now we can."

David Reichman, a professor of chemistry at Columbia University who was not involved in this research, considers the new findings "a very important contribution to the singlet fission literature. Via a synergistic combination of modeling, crystal engineering, and experiment, the authors have provided the first systematic study of parameters influencing fission rates," he says. Their findings "should strongly influence design criteria of fission materials away from goals involving molecular packing and toward a focus on the electronic energy levels of selected materials."

More information: A transferable model for singlet-fission kinetics, *Nature Chemistry* (2014) DOI: 10.1038/nchem.1945

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