# Solar cell mystery solved, expected to greatly increase efficiency

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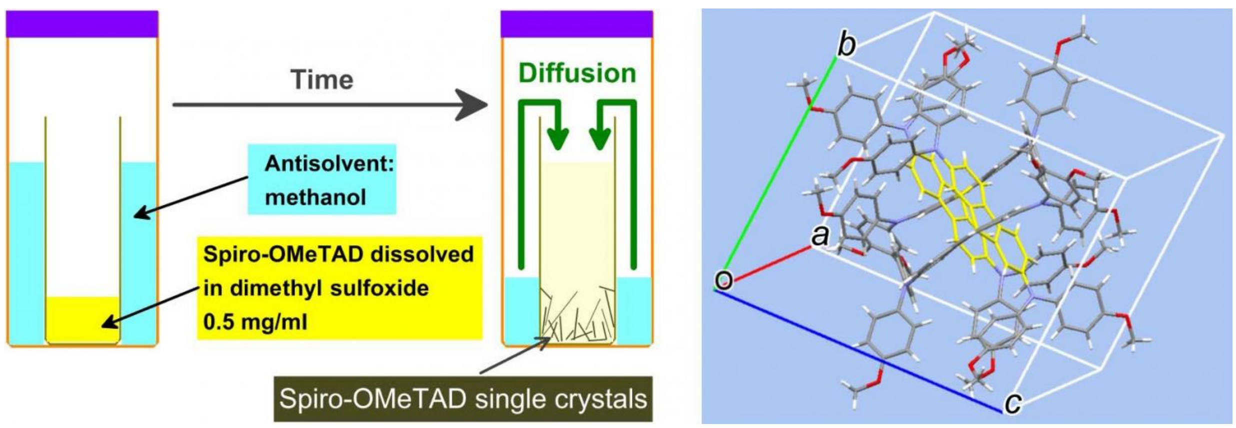


(Left) The set-up used to grow single crystals of spiro-OMeTAD, based on antisolvent vapor-assisted crystallization. (Right) Single crystal structure of spiro-OMeTAD. Credit: Shi, et al. ©2016 AAAS

(Phys.org)—For the past 17 years, spiro-OMeTAD, has been keeping a secret. Despite intense research efforts, its performance as the most commonly used hole-transporting material in perovskite and dye-sensitized solar cells has remained stagnant, creating a major bottleneck for improving solar cell efficiency. Thinking that the material has given all it has to offer, many researchers have begun investigating alternative materials to replace spiro-OMeTAD in future solar cells.

But in a new study published in *Science Advances*, Dong Shi *et al.* have taken a closer look at spiro-OMeTAD and found that it still has a great deal of untapped potential. For the first time, they have grown single crystals of the pure material, and in doing so, they have made the surprising discovery that spiro-OMeTAD's single-crystal structure has a hole mobility that is three orders of magnitude greater than that of its thin-film form (which is currently used in solar cells).

"This paper reports a major breakthrough for the fields of perovskite and solid-state dye-sensitized solar cells by finally clarifying the potential performance of the material and showing that improving the crystallinity of the hole transport layer is the key strategy for further breakthroughs in device engineering of these solar cells," Osman Bakr, a professor of engineering at King Abdullah University of Science and Technology (KAUST) in Saudi Arabia and leader of the study, told *Phys.org*.

The findings suggest that, at least in the short term, the time-consuming process of designing and synthesizing radically new organic hole conductors as replacements to spiro-OMeTAD may not be necessary.

In general, perovskite solar cells and dye-sensitized solar cells are made of three critical layers. Two of these layers—the electron-transporting layer and the light-absorbing layer—are well-understood structurally. However, the mesoscale packing structure of the hole-transporting layer, which is usually spiro-OMeTAD, has so far eluded researchers, and consequently its charge transport mechanisms have remained a mystery.

In the new study, the researchers figured out a way to grow pure single crystals of spiro-OMeTAD by dissolving the spiro-OMeTAD in a carefully chosen solvent. They then placed this vial inside a larger vial containing an antisolvent, in which spiro-OMeTAD does not dissolve as well, and allowed the antisolvent vapor to slowly diffuse into the inner vial. Eventually the solution in the inner vial becomes supersaturated, so that not all of the spiro-OMeTAD can stay dissolved, causing the spiro-OMeTAD to crystallize. The researchers then performed a variety of measurements on the crystals to investigate their charge transport mechanisms and other properties.

The results are much more encouraging than expected, in many ways running contrary to the conventional wisdom based on the material's large-scale structure, which suggested that the material had reached its limits.

Although the method used here to grow single crystals cannot be performed at a large scale, the researchers predict that similar methods that use an antisolvent to trigger crystallization could be used to enhance the crystallinity of the thin-layer spiro-OMeTAD, improving its hole mobility in order to make more efficient solar cells.

"These astonishing findings open a new direction for the development of perovskite solar cells and dye-sensitized solar cells by showing the still untapped potential of spiro-OMeTAD," Bakr said. "They unravel a key mystery that has confounded the photovoltaic community for the last 17 years."

**More information:** Dong Shi, et al. "Spiro-OMeTAD single crystals: Remarkably enhanced charge-carrier transport via mesoscale ordering." *Science Advances*. DOI: 10.1126/sciadv.1501491

**Abstract**
We report the crystal structure and hole-transport mechanism in spiro-OMeTAD [2,2′,7,7′-tetrakis(N,N-di-p-methoxyphenyl-amine)9,9′-spirobifluorene], the dominant hole-transporting material in perovskite and solid-state dye-sensitized solar cells. Despite spiro-OMeTAD's paramount role in such devices, its crystal structure was unknown because of highly disordered solution-processed films; the hole-

transport pathways remained ill-defined and the charge carrier mobilities were low, posing a major bottleneck for advancing cell efficiencies. We devised an antisolvent crystallization strategy to grow single crystals of spiro-OMeTAD, which allowed us to experimentally elucidate its molecular packing and transport properties. Electronic structure calculations enabled us to map spiro-OMeTAD's intermolecular charge-hopping pathways. Promisingly, single-crystal mobilities were found to exceed their thin-film counterparts by three orders of magnitude. Our findings underscore mesoscale ordering as a key strategy to achieving breakthroughs in hole-transport material engineering of solar cells.



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