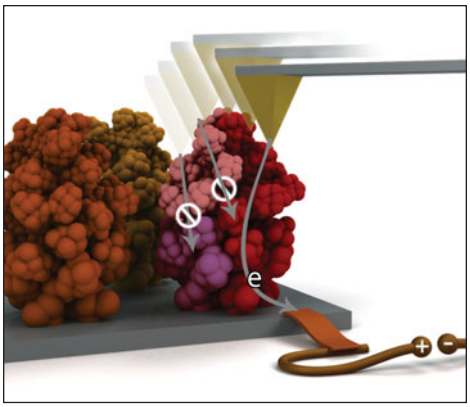
Energy Focus

Champion nanostructures identified for solar water-splitting

Researchers from École Polytechnique Fédérale de Lausanne (EPFL) and the Technion-Israel Institute of Technology (Technion) have identified "champion" nanostructures able to produce hydrogen in the most environmentally friendly and cheap manner, by simply using daylight.

In the quest for the production of renewable and clean energy, photoelectrochemical cells (PECs) constitute a sort of Holy Grail. PECs are devices able to split water molecules into hydrogen and oxygen in a single operation, under solar irradiation. "As a matter of fact, we've already discovered this precious chalice," said Michael Grätzel, director of the Laboratory of Photonics and Interfaces (LPI) at EPFL. "Today we have just reached an important milestone on the path that will lead us forward to profitable industrial applications."



Conducting atomic force microscopy examines the charge-transport properties of individual α-Fe_2O_3 (hematite) nanostructures, identifying champion nanostructures that produce solar hydrogen.

As reported in the July 7 online edition of *Nature Materials* (DOI: DOI: 10.1038/NMAT3684), EPFL researchers, working with Avner Rothschild from the Technion, have accurately characterized the iron oxide nanostructures to be used in order to produce hydrogen at the lowest possible cost. "The whole point of our approach is to use an exceptionally abundant, stable, and cheap material: rust," said Scott C. Warren, first author of the article who is now an assistant professor at the University of North Carolina at Chapel Hill.

By analogy with those solar cells that achieve record performance—so-called "champion" solar cells—the researchers have developed a process for identifying champion nanostructures within water-splitting electrodes. By characterizing the structure of the aggregates of α-Fe_2O_3 (hematite) particles, and correlating this with their charge-transport characteristics, Grätzel's research team was able to precisely characterize the movement of the electrons through the nanostructures, which were laid on electrodes during the manufacturing process. "These measures have helped us understand the reason why we get performance differences depending on the electrodes manufacturing process," said Grätzel.

Using dark-field transmission electron microscopy in combination with conducting atomic force microscopy, the researchers assessed the type of grain boundary which has the greatest influence on charge-carrier transport. "The majority carrier transport is limited primarily by high-angle grain boundaries rather than low-angle grain boundaries and imply that potential barriers form at many or most of the high-angle grain boundaries," they reported.

By comparing several electrodes, whose manufacturing method is now mastered, scientists were able to identify the "champion" structure. By replicating that nanostructure across an entire electrode, the researchers succeeded in producing electrodes that split water with a record photocurrent. A 10 × 10 cm prototype has been produced and its effectiveness is in line with expectations. The next step will be the development of the industrial process to large-scale manufacturing.

Evidently, the long-term goal is to produce hydrogen—the fuel of the future—in an environmentally friendly and especially competitive way. For Grätzel, "current methods, in which a conventional photovoltaic cell is coupled to an electrolyzer for producing hydrogen, cost €15 per kilo at their cheapest. We're aiming at a €5 charge per kilo."

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Bifunctional poly(vinylpyrrolidone) binders enhance lithium sulfide cathode performance

Intercalation cathodes used in current lithium-ion batteries have a theoretical capacity of approximately 300 mA h g^{-1}. While this is sufficient for most commercial handheld electronics, it limits the widespread use of lithium-ion batteries in large-scale applications such as zero-emission electric vehicles. Although alternative next-generation cathode materials such as sulfur and fully lithiated sulfur (Li_2S) demonstrate impressive theoretical capacities of 1673 mA h g^{-1} and 1166 mA h g^{-1}, respectively, the structural stability and long-term cycling performance of these electrodes are still unexplored.

In the September issue of *Chemical Science* (DOI: 10.1039/c3sc51476e; p. 3673), a group of researchers from Stanford University, California, and Beihang University, Beijing, report improved structural stability and cycling of Li_2S cathodes through the use of a bifunctional binder. Since previous studies have shown that compatible binders can significantly impair the overall performance of the electrode, Yi Cui's group at Stanford and their collaborators focused on finding a new binder. This would replace the commonly used poly(vinylidene fluoride) (PVDF) for sulfur cathodes that displays strong affinity to Li_2S and lithium polysulfides (Li_2S_n, $4 \leq n \leq 8$). By using *ab initio* simulations to screen various functional groups often found in macromolecular binders and their bind-

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