Demonstrating improved performance of transition metal oxide based organic photovoltaics

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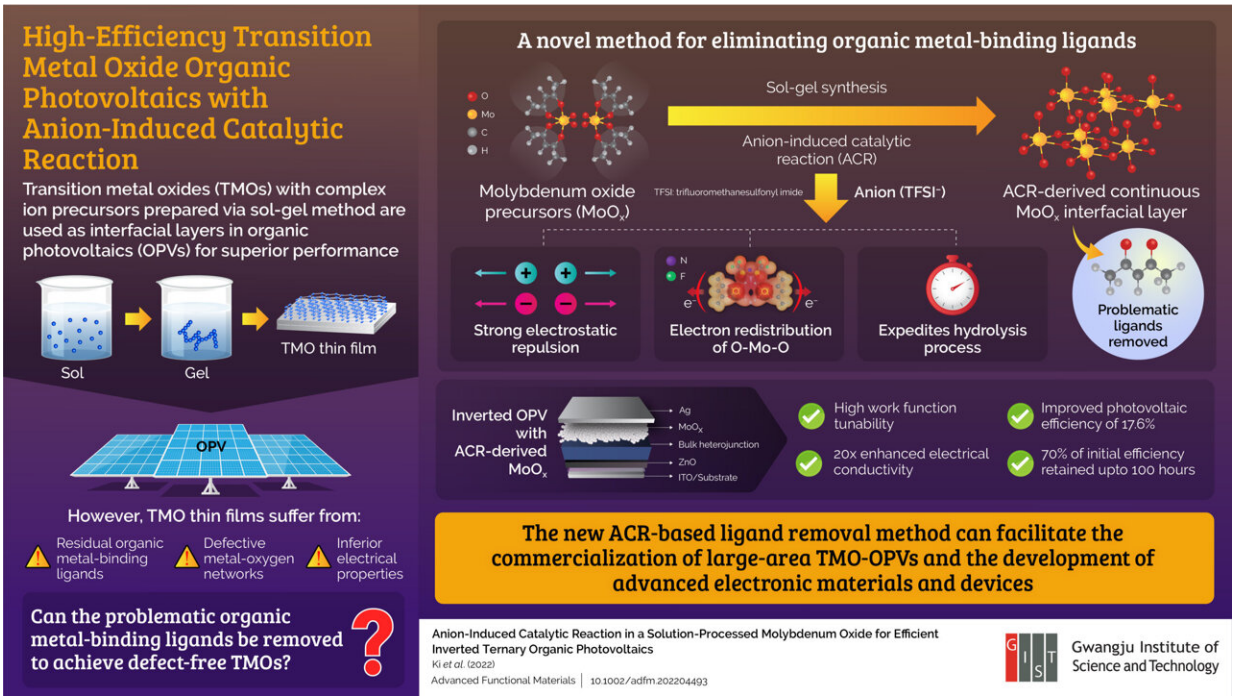

Researchers from GIST report ACR as an effective way of removing unwanted ligands and improving the efficiency of organic photovoltaics (OPVs) with a transition metal oxide (TMO) interfacial layer. Credit: Kwanghee Lee from Gwangju Institute of Science and Technology, Korea

Harnessing the power of the sun and converting it into electricity using

photovoltaic solar cells is one of the top contenders for combating the current energy crisis. To this end, researchers have developed organic photovoltaics (OPVs) with transition metal oxide (TMO) thin-film interfacial layers as a cost-effective alternative to commercial silicon solar cells.

OPVs are known for their excellent photochemical properties and low-cost mass producibility. However, the TMO layer often suffers from a degraded electrical conductivity owing to the presence of lingering organic metal-binding ligands generated during their synthesis. This greatly limits the OPVs from reaching their full potential.

A team of researchers led by Prof. Kwanghee Lee from Gwangju Institute of Science and Technology, Korea found a way to overcome this challenge. The team demonstrated a simple and effective way of eliminating the residual organic metal-binding ligands from molybdenum oxide (MoO_x) precursor at room temperature using a technique called "anion-induced catalytic reaction" (ACR).

This breakthrough was published in the journal *Advanced Functional Materials*.

When asked about the rationale behind the study, Prof. Lee says, "While OPVs with TMO thin films are headed towards power conversion efficiencies as high as 19%, the organic metal-binding ligands left behind the after sol-gel synthesis act like a double-edged sword, helping with the formation of the TMO thin films but deteriorating their properties as well. So, we aimed to find a way to eliminate the unwanted ligands after the synthesis process."

Accordingly, the team prepared a TMO thin film using an organic ligand-containing ionic compound and an MoO_x-based precursor by introducing ACR alongside the hydrolysis and condensation steps that take place

during the sol-gel method. X-ray analysis and density functional theory calculations revealed that ACR induced a strong electrostatic repulsion via low-level anions, which expedited the hydrolysis process and resulted in a quick removal of the organic-metal binding ligands at room temperature.

The team then prepared an inverted OPV configuration using the ACR-derived MoO_x thin film to test its electrical properties. To their delight, they observed a 20-fold enhancement in the film's electrical conductivity along with an excellent work function tunability compared to pristine MoO_x. Further, the inverted OPV configuration showed 17.6% improved efficiency, with over 70% retention of the initial efficiency for up to 100 hours.

This novel strategy could not only ensure a superior light-to-electricity conversion efficiency required for commercialization but also enable energy-efficient mass production of next-generation OPV solar cells. "We strongly believe that the insights provided by our findings will open up new horizons in the production of large-area, wearable, flexible, and printable electronics," says Prof. Lee.

More information: Taeyoon Ki et al, Anion-Induced Catalytic Reaction in a Solution-Processed Molybdenum Oxide for Efficient Inverted Ternary Organic Photovoltaics, *Advanced Functional Materials* (2022). DOI: 10.1002/adfm.202204493

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