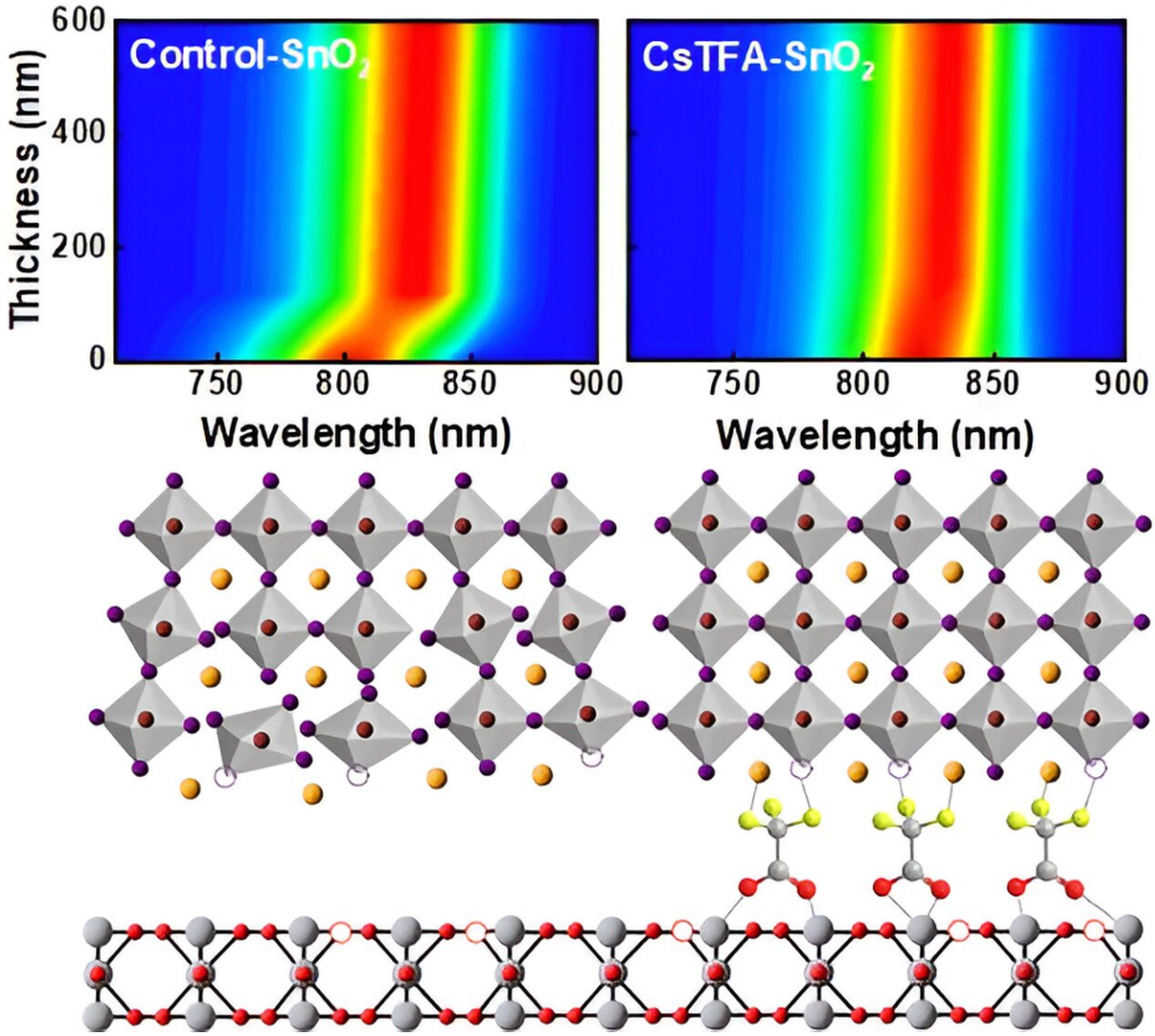
Bidirectional coordinator enhances ion arrangement in perovskite solar cells

September 10 2024, by JooHyeon Heo



Overall schematic illustration of the study. Credit: *Energy & Environmental Science* (2024). DOI: 10.1039/D4EE02017K

A joint research team from the School of Energy and Chemical Engineering and the Department of Chemistry at UNIST has addressed critical challenges in perovskite solar cell (PSC) production, significantly enhancing both their efficiency and stability, which is expected to further bolster their commercialization potential.

Led by Professors Jin Young Kim, Dong Suk Kim, and Geunsik Lee, the team successfully achieved precise control over ion arrangement and reduced structural irregularities by incorporating a bidirectional coordinator between the perovskite photoactive layer and the electron transport layer.

The work is published in the journal *Energy & Environmental Science*.

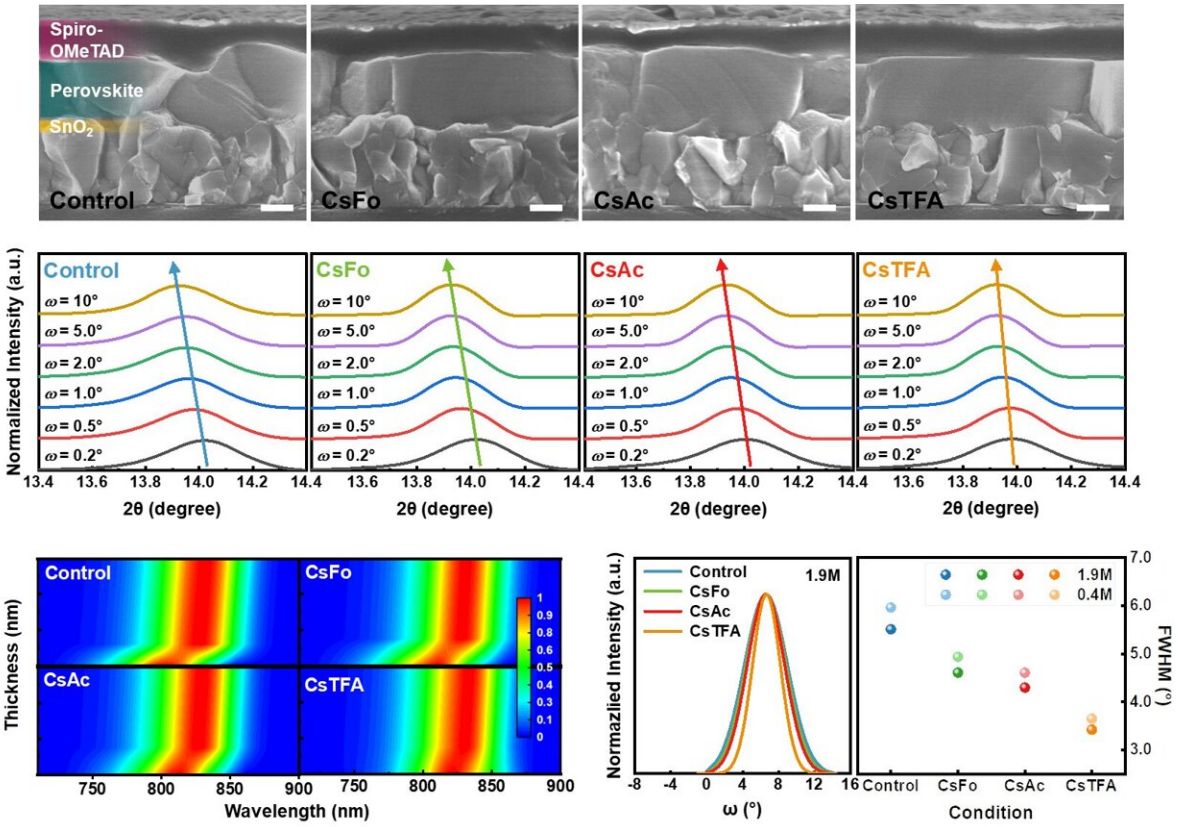
Despite their high efficiency and low manufacturing costs, perovskite solar cells have faced obstacles to commercialization due to various defect-related issues. The research team introduced trifluoroacetate (TFA^-) ions between the perovskite layer and the tin oxide substrate, which serves as the electron transport layer (ETL), to mitigate these defects.

The carboxylate group ($-COO^-$) of TFA^- firmly bonds with the tin oxide, enhancing structural stability. Simultaneously, the organic head group ($-CF_3$) effectively reduces defects through bidirectional molecular tuning that interacts with the perovskite layer.

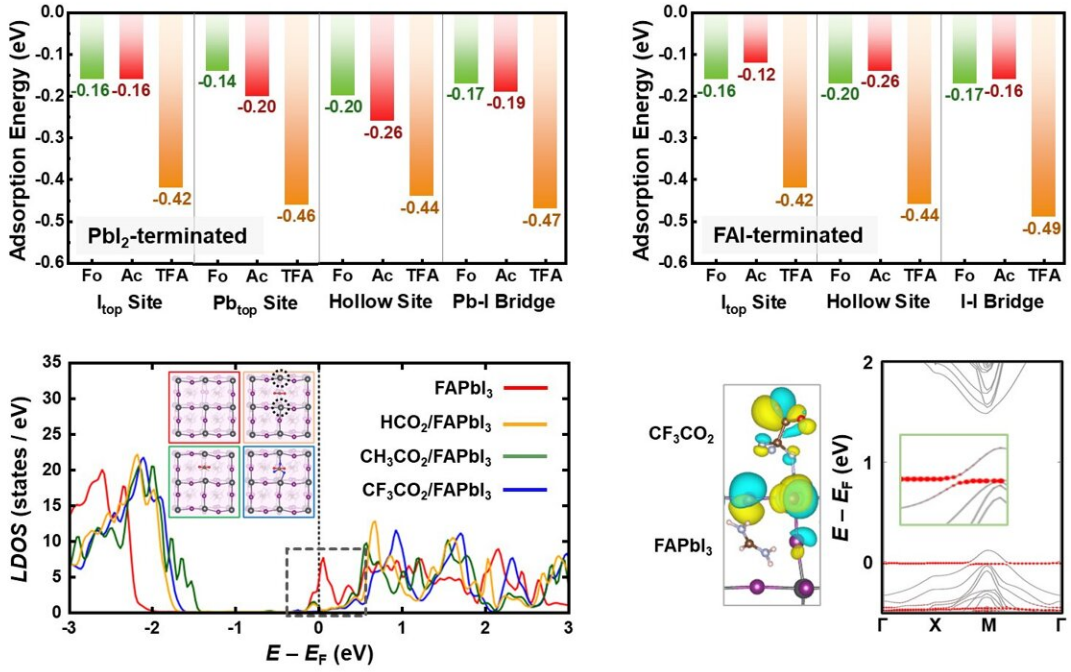
This approach allowed the research team to control the irregular structure of the perovskite thin film, substantially improving charge carrier mobility.

The resulting perovskite films, characterized by the absence of buried

interfaces and minimized tensile strain, achieved a remarkable power conversion efficiency (PCE) of 25.60%. Moreover, the unencapsulated device maintained over 80% of its initial PCE even under prolonged light exposure after 1,000 hours.



(a) Cross-sectional SEM images of the perovskite films deposited on the control- and CsX-treated SnO_2, configured as FTO/control- and CsX-treated SnO_2/Perovskite/Spiro-OMeTAD. (b) GIXRD spectra of the perovskite films deposited on the control- and CsX-treated SnO_2 upon varying the grazing incidence angle from 0.2° to 10°. (c) Normalized PL spectra upon varying the thickness of the perovskite films deposited on the control- and CsX-treated SnO_2. (d) XRD rocking curves of the perovskite films deposited on the control- and CsX-treated SnO_2 (left). FWHM values of XRD rocking curves of perovskite films with different concentrations, 0.4 M and 1.9 M, deposited on the control- and CsX-treated SnO_2 (right).



Density functional theory calculation results. Credit: *Energy & Environmental Science* (2024). DOI: 10.1039/D4EE02017K

Professor Dong Suk Kim remarked, "This groundbreaking bidirectional coordination strategy reveals a promising pathway to enhance high efficiency and confront the persistent challenge of addressing long-term stability concerns. This achievement will further enhance the commercialization potential of PSCs."

More information: Jaehwi Lee et al, Constructing orderly crystal orientation with a bidirectional coordinator for high efficiency and stable perovskite solar cells, *Energy & Environmental Science* (2024). DOI: 10.1039/D4EE02017K