Molecular ferroelectrics drive two-dimensional thin film solar cells

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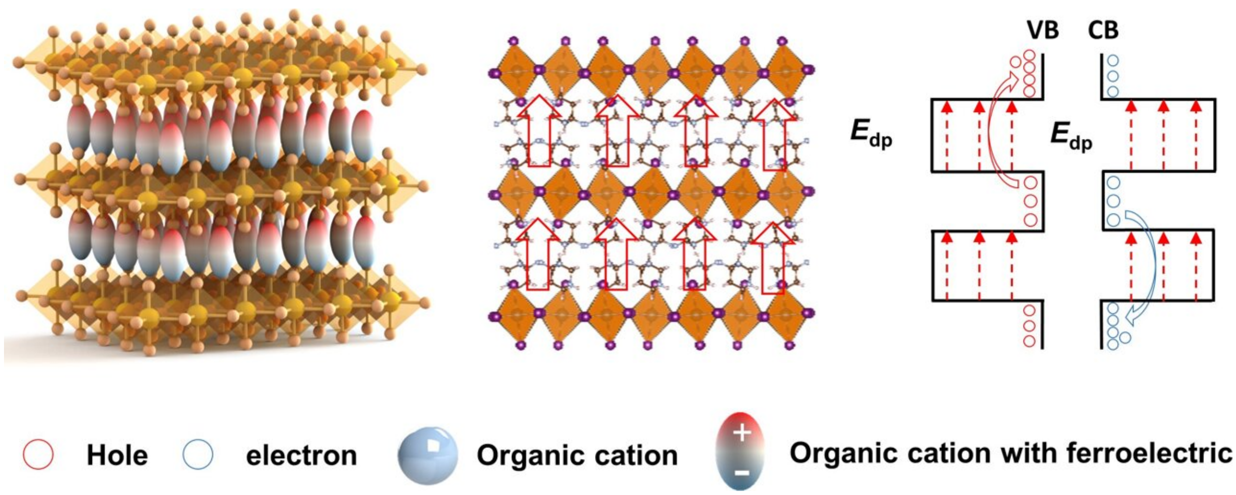

Schematic diagram of the 2D molecular ferroelectric structure, the ferroelectricity originates from the directional arrangement of organic cations, the arrow represents the depolarization field. Credit: Science China Press

Two-dimensional (2D) perovskite thin films possess diverse tunability, excellent optoelectronic properties and superior long-term stability, which are of great significance for high performance of perovskite solar cells. This study was led by Professor Guifu Zou from College of Energy, Soochow Institute for Energy and Materials Innovations, Soochow University.

"The biggest obstacle to achieving high-performance 2D perovskite solar cells is the inferior out-of-plane charge transport caused by the alternating arrangement of inorganic frameworks and organic space layers, also known as multiple quantum well electronic structures," says Professor Zou.

"Over the past decade, molecular ferroelectrics with perovskite structure have been extensively studied due to excellent characteristics such as strong saturation polarization, high Curie temperature, multiaxial properties, low preparation temperature, and narrow band gap. The polarization field in molecular ferroelectricity will be greatly helpful to improve the performance of 2D perovskite solar cells."

As documented in a new paper published today in *National Science Review*, researchers fabricated 2D perovskite solar cells based on molecular ferroelectric with large spontaneous polarization, high Curie temperature and multi-equivalent ferroelectric axes.

"The moderate band gap and high absorbance coefficient of these materials enable effective absorption of visible light. Moreover, their low crystallization temperature makes it possible to design devices with optimal energy level structures," says Chen Wang, first author of the study and a Ph.D. student in Professor Zou's team.

"The high Curie temperature, large spontaneous polarization and strong residual polarization ensure excellent ferroelectric properties at room temperature."

Studies on the photoelectric properties of molecular ferroelectrics have revealed that the depolarization field can affect the photoluminescence and interfacial energy level of the film.

The chemical environment of the constituent elements changes after polarization, indicating that the lead iodide inorganic framework might participate in the polarization process. "We hope our findings will contribute to a better understanding of the polarization process in molecular ferroelectrics," says Wang.

"What we found is that polarization fields can effectively separate and transport charges that are trapped in multiple quantum well electronic structures, resulting in improved device performance after polarization," says another Ph.D. student Lutao Li from Professor Zou's team, the co-author on the new paper.

"Under one sun illumination, the obtained 2D ferroelectric solar cells achieved an impressive performance, which is the highest open circuit voltage (1.29 V) and the best efficiency among the 2D (n=1) Ruddlesden-Popper perovskite solar cells."

Simulations of ferroelectric photovoltaic devices can aid in the understanding of the space charge region and electric potential within the p-i-n junction under the influence of polarization.

This study not only provides a solution platform for the poor out-of-plane conductivity from intrinsic multiple quantum well electronic structure limits of 2D materials, but also demonstrates a promising application for 2D molecular materials for optoelectronics.

"Thin film materials are extensively researched in the field of optoelectronics and photovoltaics, and creating desirable thin films or surpassing the limitations of 2D thin-film materials is a significant challenge. Professor Zou's innovative work bridges molecular ferroelectrics with perovskite photovoltaics, overcoming the intrinsic limits of the multiple quantum well electronic structure of 2D materials. This breakthrough has led to the demonstration of highly efficient 2D thin film solar cells," says Dr. Nilan J.B. Kamathewatta, a thin-film scientist at Intel Corporation.

"In recent years, emerging molecular ferroelectrics with unique and excellent properties have shown promising prospects in the field of ferroelectricity. These exciting developments have made ferroelectric research a hot topic once again. Professor Zou's work provides evidence for a deeper understanding of the origin of ferroelectricity in molecular ferroelectrics. I believe that this study will draw more attention from scientists to molecular ferroelectrics and further expand their applications in various fields," says Professor Rengen Xiong, Director of the Order Matter Science Research Center at Nanchang University.

"Perovskite solar cells have attracted unprecedented attention in recent years for their high power conversion efficiency, ease of fabrication, and tunable properties. In Professor Zou's study, novel molecular ferroelectrics are utilized to fabricate 2D perovskite solar cells. The introduction of ferroelectricity improved the separation and transport of out-of-plane carriers, resulting in excellent device performance. Additionally, the incorporation of ferroelectricity within the molecular ferroelectrics enhances the built-in electric field, providing innovative solutions to achieve high open-circuit voltage perovskite solar cells," according to Professor JaeJoon Lee, President of the Korean Photovoltaic Society.

The researchers are focusing on improving the efficiency of molecular ferroelectrics by exploring materials that possess lower bandgap, higher residual polarization, and other favorable properties.

"In the pursuit of achieving better performance in molecular ferroelectric solar cells, low-bandgap molecular ferroelectrics with 3D structures will be given more attention in the future. There is still much to be discovered in this field," says Professor Zou.

The Guifu Zou Research Group at Soochow University is a leading research team dedicated to exploring new frontiers in the field of thin-film materials science. In addition to their work on molecular ferroelectric materials, the group has conducted groundbreaking research in the area of ultrathin film materials.

The team's research in thin film materials has focused on developing innovative methods for depositing and growing high-quality thin films with precise control over their properties. They have investigated a range of techniques to optimize the growth process and improve the properties of the resulting thin films.

One of the major accomplishments in the field of thin film materials is the development of new methods for growing complex thin films. These thin films are characterized by their high crystalline quality and excellent electrical conductivity, making them ideal for use in electronic devices and energy conversion applications.

In addition to their research on thin films, the group has also explored other types of ultrathin films, such as 2D films and other atomically-thin films. Their research has led to many important discoveries and advancements in these areas, including insights into the growth mechanisms of ultrathin films and new physics for specific applications.

Overall, the Guifu Zou Research Group's research in thin film materials represents an important contribution to the field of materials science. Their work has helped to advance our understanding of thin film growth and optimization, and has opened up new possibilities for the development of novel materials and technologies.

More information: Chen Wang et al, Two-dimensional (n = 1) Ferroelectric Film Solar Cells, *National Science Review* (2023). DOI: 10.1093/nsr/nwad061

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