Cause of external pressure-induced performance deterioration in solar cells identified

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Dr. Jung-hoon Lee of the KIST is currently following up on the research by developing materials optimized for hybrid Perovskite solar cells. Credit: Korea Institue of Science and Technology(KIST)

A team, led by Dr. Jung-hoon Lee of the Computational Science Research Center of the Korea Institute of Science and Technology (KIST), recently collaborated with a team, led by Professor Jeffrey B. Neaton from the UC Berkeley Department of Physics, to develop a theoretical explanation for the structural changes and metallization that take place when hybrid (organic metal halide) perovskite solar cells are exposed to external pressure. The explanation announced by the two teams is attracting much attention from related academic and industrial circles

Today, solar cells are not only used in our everyday lives, but are also used in extreme conditions such as atmospheric, space, desert, and maritime environments. Hybrid perovskite solar cells [comprised of organic metals, halide (I) and lead (Pb): $(CH_3NH_3)PbI_3$] are highly efficient and involve low production costs. These cells are promising, next-generation solar cells that can potentially be used to replace costly conventional silicon solar cells. Recognizing this potential, many researchers have been trying to engineer highly efficient hybrid perovskite solar cell materials that are able to operate normally even in extreme conditions.

However, phase transition from the orthorhombic to cubic structures has been reported in hybrid perovskite solar cells, when the cells are exposed to high external pressure. Metallization has also been reported, wherein electricity flows within the element and renders it unable to function properly. These changes under pressure have been major hurdles to the commercialization of hybrid perovskite solar cells. Hybrid perovskite solar cells with modified structures and characteristics are unable to convert solar radiation into electric energy. This indicates that external pressure substantially deteriorates the performance of the solar cells. However, prior to this study, the cause of the deterioration had not yet been clearly identified.

The joint KIST-UC Berkeley research team used a supercomputer and quantum mechanical theory (density functional theory) to theoretically explain the pressure-induced structural changes (phase transition) and metallization in hybrid perovskite solar cells. By accurately predicting the phase transition pressure, the research team found that the cubic structure becomes more favorable for organic molecules than the original orthorhombic structure under high pressure, leading to the pressure-induced phase transition. Further, the research team theoretically demonstrated that lead atoms in the hybrid perovskite cells interact under high pressure, leading to metallization, which turns the solar cells into conductors and causes electricity to flow through them.

The KIST-UC Berkeley team is the first research team that has been able to identify the cause of the performance deterioration in hybrid perovskite solar cells under external pressure. Dr. Jung-hoon Lee of KIST is currently following up on the research by developing materials optimized for hybrid perovskite solar cells. In particular, Dr. Lee is researching organic molecules in which stabilities are insensitive to different inorganic structures, and is looking for a replacement for the lead used in the cells, which is both the cause of the metallization and a major contributor to environmental destruction. Lee's research is expected to spur the development of next-generation solar cells that will eventually replace silicon solar cells.

"We expect that our study will provide new theoretical guidelines for the future development and optimization of high-performance hybrid perovskite solar cells," stated Dr. Jung-Hoon Lee of the KIST. "We hope our results contribute to establishing hybrid perovskite solar cells as a next-generation solar cell to replace silicon solar cells."

More information: Jung-Hoon Lee et al, Origins of the Pressure-Induced Phase Transition and Metallization in the Halide Perovskite $(CH_3NH_3)PbI_3$, *ACS Energy Letters* (2020). DOI: 10.1021/acsenergylett.0c00772

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