Photovoltaic Enhancement Accompanied by Polar-instability: $BiFeO_3$ vs $MAPbI_3$

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Ferroelectric materials for photovoltaics have sparked interest recently due to their high photovoltages. However, the relatively low photo-current and power conversion efficiency limit their potential applications. The recently discovered hybrid perovskite $MAPbI_3$, in which a giant photostrictive effect similar to that in ferroelectric oxides has been observed [1], offers a potential avenue to improve the ferroelectric photovoltaic effect.

It was suggested that the dynamic polar *A*-site group in $MAPbI_3$ play a critical role for their ultra-long carrier lifetime. We have investigated the hypothesis using an inorganic perovskite, $BiFeO_3$. By engineering its *A* site via La doping, $BiFeO_3$ displays large photovoltaic enhancement and polar-instability simultaneously. The improvement is attributed to the longer photocarrier lifetime as revealed by optical measurements and supported by theoretical calculations. Such polar-instability-driven band structure tuning may guide future materials design to maintain the momentum of photovoltaic efficiency increase. In addition, we investigate the effects on the carrier lifetime from a subtle direct to indirect band gap transition induced by A-site doping.

Reference:

[1], "Giant Photostriction in Organic-Inorganic Lead Halide Perovskites", Yang Zhou[†], Lu You[†], Zhiliang Ku, Hongjin Fan, Shiwei Wang, Daniel Schmidt, Andrivo Rusydi, Lei Chang, Le Wang, Peng Ren, Liufang Chen, Guoliang Yuan, and Junling Wang[*], Nature Communications 7:11193, doi: 10.1038/ncomms11193, (2016).

[2], "Photovoltaic enhancement accompanied by polar-instability", Lu You, Fan Zheng, Liang Fang, Yang Zhou, Liang Z. Tan, Zeyu Zhang, Guohong Ma, Daniel Schmidt, Andrivo Rusydi, Le Wang, Peng Ren, Shiwei Wang, Lei Chang, Andrew M. Rappe[*], Junling Wang[*], in preparation (2017).