The Existence and Impact of Persistent Ferroelectric Domains in $MAPbI_3$

Scientific Achievement

Methylammonium lead iodide ($MAPbI_3$) exhibits exceptional photovoltaic performance. But a significant controversy remains over the existence and impact of ferroelectricity on the photovoltaic response. We confirm ferroelectricity in $MAPbI_3$ single crystals and demonstrate mediation of the electronic response by ferroelectric domain engineering.

Significance and Impact

This work also demonstrates how to control the ferroelectricity response in $MAPbI_3$ and its influence on the optoelectronic response—such as measurable changes in Fermi level position, conductivity, response to an electrical probe, and the rate at which it degrades—suggesting that domain engineering is a viable route to increased performance and stability.

Research Details

Theory: First-principles calculations were performed using the projector augmented wave method as implemented in the Vienna Ab Initio Simulation Package. Structures were relaxed using the standard parameters of the Materials Project.

Experimental: Because of controversial reports in the literature, an extensive set of characterization tools was employed to examine large single crystals of $MAPbI_3$. The tools included X-ray crystallography, piezoresponse force microscopy, electric response force microscopy, scanning microwave impedance spectroscopy, band-excitation piezoresponse force microscopy with contact Kelvin probe force microscopy, X-ray photoelectron spectroscopy, electrical characterization, and Berlincourt d_{33} measurements.

Rayleigh Response for $MAPbI_3$ Single Crystal

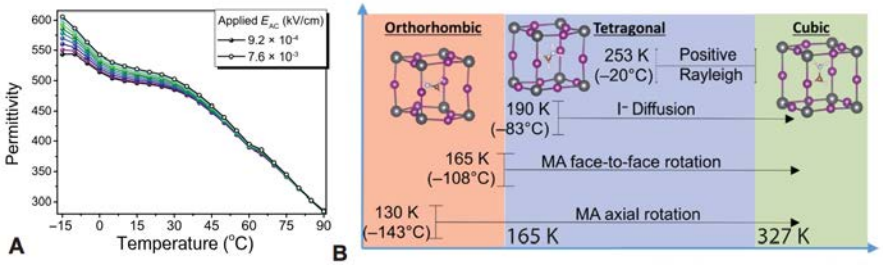

Figure 1. (**A**) Rayleigh response, determined from the *E*AC dependence of the permittivity. (**B**) Schematic of the material structure, temperature dependence of the global phase transitions, possible mechanisms of structural modification, and Rayleigh response in $MAPbI_3$.

Domain Formation on Poling in $MAPbI_3$ Crystal

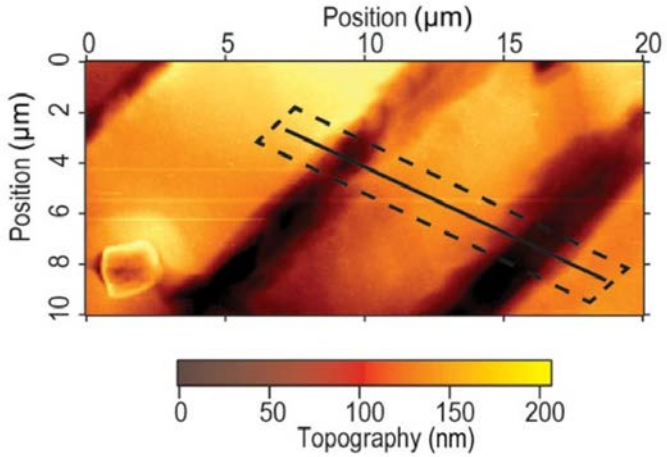

Figure 2. The AFM topography of domain lines.

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