Real-Space Imaging of the Atomic Structure of Organic-Inorganic Perovskite

Robin Ohmann, Luis K. Ono, Hui-Seon Kim, Haiping Lin, Michael V. Lee, Youyong Li*, Nam-Gyu Park*, and Yabing Qi*

1Energy Materials and Surface Sciences Unit (EMSS), Okinawa Institute of Science and Technology Graduate University (OIST), 1919-1 Tancha, Onna-son, Okinawa 904-0495, Japan. 2School of Chemical Engineering and Department of Energy Science, Sungkyunkwan University (SKKU), Suwon 440-746, Korea. 3Institute of Functional Nano and Soft Materials (FUNSOM), Soochow University, Suzhou 215123, P. R. China.

E-mail: *Yabing.Qi@OIST.jp, *npark@skku.edu, *yyli@suda.edu.cn

Organic–inorganic perovskite is a promising class of materials for photovoltaic applications and light emitting diodes. However, so far commercialization is still impeded by several drawbacks. Atomic-scale effects have been suggested to be possible causes, but an unequivocal experimental view at the atomic level is missing. Here, we present a low-temperature scanning tunneling microscopy study of single crystal methylammonium lead bromide CH$_3$NH$_3$PbBr$_3$. Topographic images of the in situ cleaved perovskite surface reveal the real-space atomic structure. Compared to the bulk we observe modified arrangements of atoms and molecules on the surface. With the support of density functional theory we explain these observations by surface reconstruction and a substantial interplay of the orientation of the polar organic cations (CH$_3$NH$_3$)$^+$ with the position of the hosting anions. This interplay leads to structurally and electronically distinct domains with ferroelectric and antiferroelectric character. We further demonstrate local probing of defects, which may also impact device performance.

Figure 1: Atomic resolution STM images of ferroelectric (left) and antiferroelectric (right) surface domains of CH$_3$NH$_3$PbBr$_3$ and corresponding model (center).

Reference: