Viernes 20 de marzo, 12:00 en el Salón de Grados de CATEPS (Bloque amarillo, 2ª planta)

Seminario “Atomic-scale microstructure of lead halide perovskite thin films”

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Studying photoactive hybrid perovskites by transmission electron microscopy (TEM) has proved particularly challenging due to the large electron energies typically employed in these studies. In particular, the very close structural relationship between a number of crystallographic orientations of the pristine perovskite and lead iodide has resulted in severe ambiguity in the interpretation of EM-derived information, severely impeding the advance of atomic resolution understanding of the materials.

In this talk, I will outline how to reliably study hybrid organic-inorganic perovskite materials using electron microscopy. With the ability to image the pristine phase of these beam-sensitive materials, we are able to obtain highly localised crystallographic information about technologically relevant materials. Using low-dose selected area electron diffraction, I will show how mixing the archetypal $CH(NH_2)_2PbI_3$ ($FAPbI_3$) and $CH_3NH_3PbI_3$ ($MAPbI_3$) improves solar cell device performance through the elimination of twin domains and stacking faults.

Using a careful low-dose scanning TEM (STEM) protocol, we are also able to image these materials in their thin-film form with atomic resolution. [Our images enable a wide range of previously undescribed phenomena to be observed, including a remarkably highly ordered atomic arrangement of sharp grain boundaries and coherent perovskite/PbI_2 interfaces, with a striking absence of long-range disorder in the crystal. These findings explain why inter-grain interfaces are not necessarily detrimental to perovskite solar cell performance, in contrast to what is commonly observed for other polycrystalline semiconductors. Additionally, we observe aligned point defects and dislocations that we identify to be climb-dissociated and confirm the room-temperature phase of $CH(NH_2)_2PbI_3$ to be cubic. We further demonstrate that degradation of the perovskite under electron irradiation leads to an initial loss of $CH(NH_2)^{2+}$ ions, leaving behind a partially unoccupied, but structurally intact, perovskite lattice, explaining the unusual regenerative properties of partly degraded perovskite films. Our findings thus provide a significant shift in our atomic-level understanding of this technologically important class of lead-halide perovskites.

Dr Mathias Uller Rothmann is a Natural Science Foundation of China Overseas Excellent Young Research Fellow at Foshan Xianhu Laboratory in China and has spent over ten years studying photoactive perovskites with various microscope techniques. He obtained his M.Sc. in Physics and Nanotechnology Engineering from the Technical University of Denmark and his PhD in Materials Science and Engineering at Monash University in Melbourne, Australia, which was followed by a postdoctoral researcher position at the University of Oxford. He has published several papers on electron and scanning probe microscopy and photoactive perovskites, including publications in Science and Nature Energy, and he is currently working on further developing advanced microscopy techniques to study this class of materials and their associated devices.