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Addressing perovskite stability: crafting an protective layer for sustainable solar cells with the use of synchrotron-based X-ray spectroscopy techniques

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Our research explores the possibility to enhance the stability and functionality of perovskite solar cells through the encapsulation of these materials with isomorphically substituted calcium hydroxyapatite ($Ca_{10-z}X_z(YO_4)_6(OH)_2$, where X = Ni, Fe, Cu; Y = V, P) as a transparent encapsulating layer. Building upon recent findings on the electronic structure of calcium apatites, we aim to optimise the composition and properties of the encapsulating layer to suit the requirements of potential photovoltaic applications. This encapsulation approach addresses the key challenges of perovskite degradation due to moisture and oxygen exposure, as well as mitigates the environmental hazard of lead leakage.

The project aims to explore the local environment and structure of the compounds in consideration, in particular the nature of Ca-O, P-O, Fe-O bonds, as well as the Pb-I bond, which is responsible for phase transitions in perovskite and poor stability of solar cells; establish the mechanisms of ion migration in the perovskite structure and study the dynamics of charge transfer. To achieve this, synchrotron-based techniques such as micro-X-ray fluorescence (μXRF), X-ray absorption spectroscopy (μXAS), and X-ray photoelectron spectroscopy will be integrated, in conjunction with theoretical calculations, in order to gain insight into the perovskite-apatite interface. The combination of high-resolution spectroscopic analysis and quantum mechanical modelling allows for precise control over charge dynamics, local atomic structures, and ion migration pathways within the cell.

Furthermore, the project aims to facilitate the development of a dedicated Ukrainian beamline at the SOLARIS synchrotron facility, boosting research infrastructure and expertise in Ukraine.

Type of presence

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