Contribution ID: **323** Contribution code: **P-TUE-43** Type: **Poster**

Photophysical dynamics in $(CH_3NH_3)PbX_3$ (X=Br, Cl) single crystal perovskites studied by Muon-Spin Spectroscopy

Tuesday, 30 August 2022 18:00 (20 minutes)

In our efforts to help the earth recover from ecological burnout we have been trying to bridle the sun's energy since 1954, when the first practical silicon solar cell was introduced. Today we are researching for ever higher efficiencies, while we try to make use of earth-abundant materials. Perovskite solar cells are promising candidates for next generation photovoltaic technology due to their energy gap tunability and significantly long carrier lifetime which leads to a high diffusion length.
This study focuses on ion diffusion in (CH3NH3)PbX3 (X=Br, Cl) hybrid perovskites, structures that contain moving organic cations confined in a cage structure of PbX6 octahedra. Diffusing ions can affect the local magnetic field distribution. We employ muon spin spectroscopy (μ+SR) to exploit this effect by studying the relaxation of muon spin in local electronic and nuclear fields. Single crystals were studied in a 30-340 K temperature range with and without illumination. We investigate the thermally activated regions, compare the extracted diffusion rate coefficients and activation energies. However, the dynamical structure and structural transitions of hybrid perovskites make theoretical interpretations challenging. With μ+SR we are able to detect these structural changes and study their effect on the diffusive properties of the crystals.

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Session Classification: Posters

Track Classification: Energy materials