Contribution ID: **96** Type: **Talk (20 min + 5 min discussion)**

Vacancy defects in $CsPbBr_3$

Thursday 5 December 2024 17:10 (25 minutes)

The metal halide perovskites (MHPs) are attracting intense research interest due to their excellent optoelectronic properties. The all-inorganic member $CsPbBr_3$ is of particular interest for gamma-ray detector applications and LEDs. Further, single crystals can be grown via a solution route or by a melt process, and thin films can be solution processed or produced by vapour deposition.
Here we report the results of two-component density functional theory (TC-DFT) calculations for $CsPbBr_3$ and the results from variable-energy positron annihilation lifetime spectroscopy measurements on a range of single crystal CsPbBr3 samples as well as vapour processed thin samples. The TC-DFT calculations return positron lifetime values approximately similar to those previously reported for the model MHP $MAPbI_3$. Evidence for the detection of both B-site and A-site vacancy defects is presented.

Primary author: KEEBLE, David (University of Dundee)

Presenter: KEEBLE, David (University of Dundee)

Session Classification: Positrons

Track Classification: Positrons