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Vacancy defect identification in lead halide perovskite materials

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There is intensive focus on the development of lead halide perovskite for a range of photonic devices including solar cells and gamma-ray detectors. Lead occupies the perovskite B-site where it is octahedrally coordinated by halide anions, while the larger A-site accommodates a small organic molecular ion, for example, methylammonium (MA) ($CH_3NH_3^+$). The rapid development has, in part, been attributed to reports of modest defect densities, there is nevertheless intense efforts to identify and quantify point defects in these materials. The Vacancy defects are a centrally important class hence positron annihilation spectroscopies are of directly relevance. Here we report the results of variable energy positron annihilation lifetime spectroscopy measurements performed on a range of lead halide perovskites using the mono-energetic positron source beamline at Helmholtz–Zentrum Dresden–Rossendorf. Measurements have been performed on single crystal $MAPbI_3$, $MAPbBr_3$, $MAPbCl_3$, and on formamidinium (FA) lead bromide, $FAPbBr_3$. Comparison with two-component density functional theory calculated lifetime for positron states localised at vacancy defects provide evidence for the identification of both Pb vacancy and MA-vacancies.

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