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Identification of Vacancy Defects in Lead Halide Perovskites

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Metal halide perovskites are remarkable optoelectronic materials, within a decade the photovoltaic (PV) power-conversion efficiencies have risen from a few percent to exceed 25%. Yet advance toward the theoretical Shockley-Queisser limit value has slowed and this has been attributed to defect-assisted nonradiative recombination. First-principles calculations provide detailed insight on point defect structure and electronic properties, and on their role in fundamental mechanisms that govern material performance. While experiments have clearly identified the presence of deep defects, there has been no report of an experimental microscopic identification of a point defect. Here we detect and identify the presence of Pb cation monovacancies in the prototypical CH3NH3PbI3 (MAPbI3) using positron lifetime spectroscopy supported by density function theory. Measurements on thin film and single crystal materials all exhibit positron trapping, approaching saturation, to Pb vacancy defects with a density estimated to be greater than ~ 3 x 10^15 cm-3. No trapping to MA cation vacancies was detected. These results demonstrate the capability to experimentally identify and quantify the presence of cation vacancy and vacancy cluster point defects in metal halide perovskite materials.

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