MLZ User Meeting 2022



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Type: Talk (20 min + 5 min discussion)

Identification of vacancy-related defects in photovoltaic thin films

Variable energy positron annihilation lifetime measurements and related density functional theory calculations of positron lifetimes are presented and discussed for two emerging thin film photovoltaic materials, the binary semiconductor Sb₂Se₃ and the halide perovskite MAPbI₃. Measurements on a series of Sb₂Se₃ thin film and single crystal samples are presented. DFT calculations provide evidence for the identification of Sb monovacancy defects and divacancies. Measurements on MAPbI₃ samples from three groups supported by DFT calculations provide evidence for the identification of Pb vacancy (B-site) related defects. A comparison between DFT calculated lifetime in MA containing halide perovskites with varying anion type are given and discussed. '

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