$CsPbCl_3$:Yb^{+3} STRUCTURAL ANALYSIS USING HYSCORE SPECTROSCOPY

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When Yb^{+3} ions are doped into the $CsPbCl_3$ crystal lattice the material exhibits especially effective infrared light emission during quantum splitting. Due to this property, this perovskite is a promising candidate for applications in quantum technologies, light-emitting diodes, lasers, photodetectors and solar-energy conversion. However, the lattice position occupied by Yb^{+3} ions has not been clearly established, despite its critical importance for optimizing the material's performance.

In this work, electron paramagnetic resonance (EPR) and hyperfine sublevel correlation (HYSCORE) spectroscopies, methods intended for structural analysis of materials with unpaired electrons, were employed to determine the lattice site of Yb^{+3} in $CsPbCl_3$ perovskite. Previous studies in our laboratory established key spectroscopic parameters, including the anisotropic g-factor and the hyperfine interaction associated with the Yb^{+3} center, but the structural assignment remained unresolved. Analysis of hyperfine and quadrupole interactions between the unpaired electron and surrounding Cs^{+}, Pb^{+2}, and Cl^{-} nuclei, via comparing experimental and simulated HYSCORE spectra, enabled identification of the Yb^{+3} local environment. The spectroscopic analysis indicates that Yb^{+3} ions substitute for Pb^{+2} sites within the $CsPbCl_3$ lattice rather than occupying interstitial positions or substituting Cs^{+} sites. This structural assignment provides direct insight into the local electronic environment of Yb^{+3}.