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AI-enhanced High Resolution Functional Imaging Reveals Trap States and Charge Carrier Recombination Pathways in Perovskite

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Perovskite thin films are promising for optoelectronic applications such as solar cells and LEDs, but defect formation remains a major challenge. In our study, we combine high-resolution functional intensity modulation two-photon microscopy1 with AI-enhanced data analysis to gain a deeper understanding of defect-related trap states in perovskite microcrystals2,3.

Based on methylammonium lead bromide ($MAPbBr_3$) perovskite microcrystalline films, we developed a comprehensive carrier recombination model that captures the equilibrium dynamics of both excitonic and electron–hole pair photoluminescence (PL) emission. By systematically varying model parameters, we generated a large dataset of temperature-dependent, intensity-modulated PL spectra to train and optimize a machine learning regression framework for intensity-modulation two-photon microscopy (ML-IM2PM). To improve model performance and generalizability, a balanced classification sampling strategy was implemented during the training phase.

The resulting regression-chain model accurately predicts key physical parameters—exciton generation rate (G), initial trap concentration (N_TR), and trap activation energy (E_a)—across a spatially resolved 576-pixel map. These outputs were then used to solve a system of coupled ordinary differential equations (ODEs), enabling pixel-by-pixel simulations of carrier dynamics and recombination behavior under steady-state photoexcitation.

The simulations reveal pronounced spatial heterogeneity in exciton, electron, hole, and trap populations, as well as in both radiative and nonradiative recombination rates. Correlation analysis delineates three distinct recombination regimes: (i) a trap-filling regime dominated by nonradiative recombination, (ii) a transitional crossover regime, and (iii) a band-filling regime characterized by enhanced radiative efficiency. A critical trap density threshold of approximately 10^{17} cm^{-3} marks the boundary between these regimes.

Together, these findings establish ml-IM2PM as a robust platform for high-resolution, quantitative diagnosis of charge carrier dynamics in perovskite materials, offering valuable insights for targeted defect passivation and device optimization strategies.

Acknowledgements

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References

1 Q. Shi, P. Kumar, and T. Pullerits, ACS Phys. Chem. Au., 2023, 3, 467–476.

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3 Q. Shi and T. Pullerits, Energy & Environmental Materials, p.e70062.

Broad physics domain

Charge carrier recombination, Perovskite, Traps properties

AI/ML technique(s) to be presented

Regression Chain- Extra Tree.

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