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

Qi Shi[1], Tõnu Pulletits[1,*]

[1]*The Division of Chemical Physics, NanoLund, Department of Chemistry, Lund University, Kemicentrum Naturvetarevägen 16, 223 62 Lund, Sweden*
*tonu.pullerits@chemphys.lu.se

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 microscopy[1] with AI-enhanced data analysis to gain a deeper understanding of defect-related trap states in perovskite microcrystals.

Based on methylammonium lead bromide ($MAPbBr_3$) perovskite microcrystalline films, our carrier recombination dynamic model comprehensively includes the equilibrium dynamics of exciton and electron-hole pair photoluminescence (PL) emission (see Figure 1a). By varying parameters of the model, a large pool of temperature-dependent intensity modulation PL spectra can be simulated, which have been used for optimizing the machine learning regression model for intensity modulation two photon microscopy (ml-IM2PM)[2] (see Figure 1b). Furthermore, the ml-IM2PM allows for micro-meter scale maps of the spatial heterogeneity of defect properties and their impact on carrier recombination pathways in $MAPbBr_3$ perovskite microcrystalline films (see Figure 1c). In regions where bromide interstitial Br_i defects predominate, the effective trap density is relatively higher, leading to significant non-radiative recombination losses. Conversely, regions dominated by vacancy defects, V_{Pb} and V_{Br}, exhibit lower effective trap densities, which result in a notable enhancement of PL emission from free electron hole pairs. These results highlight the potential of defect suppression, such as surface passivation and controlled crystallization, to optimize the performance and stability of perovskite semiconductors. Our study suggests that AI-enhanced high resolution functional imaging hold promise for advancing the study of various photoactive devices.

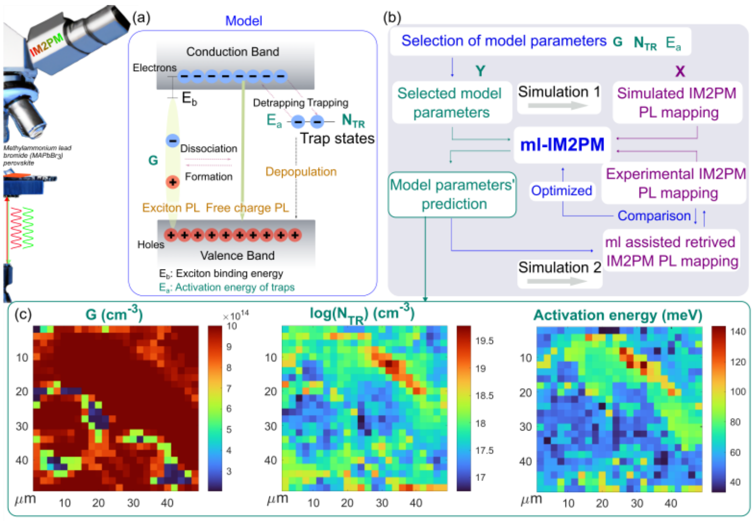

Figure 1 (a) carrier recombination dynamic model. (b) machine learning regression analysis of intensity modulation two-photon microscopy (ml-IM2PM). (c) micro-meter scale maps of the parameters (generation of excitons (G), total trap concentration (N_{TR}), and trap activation energy (E_a)).

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References

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