Supplementary Information for

Intricate carrier dynamics of bismuth halide perovskites: localized excitons and polarons

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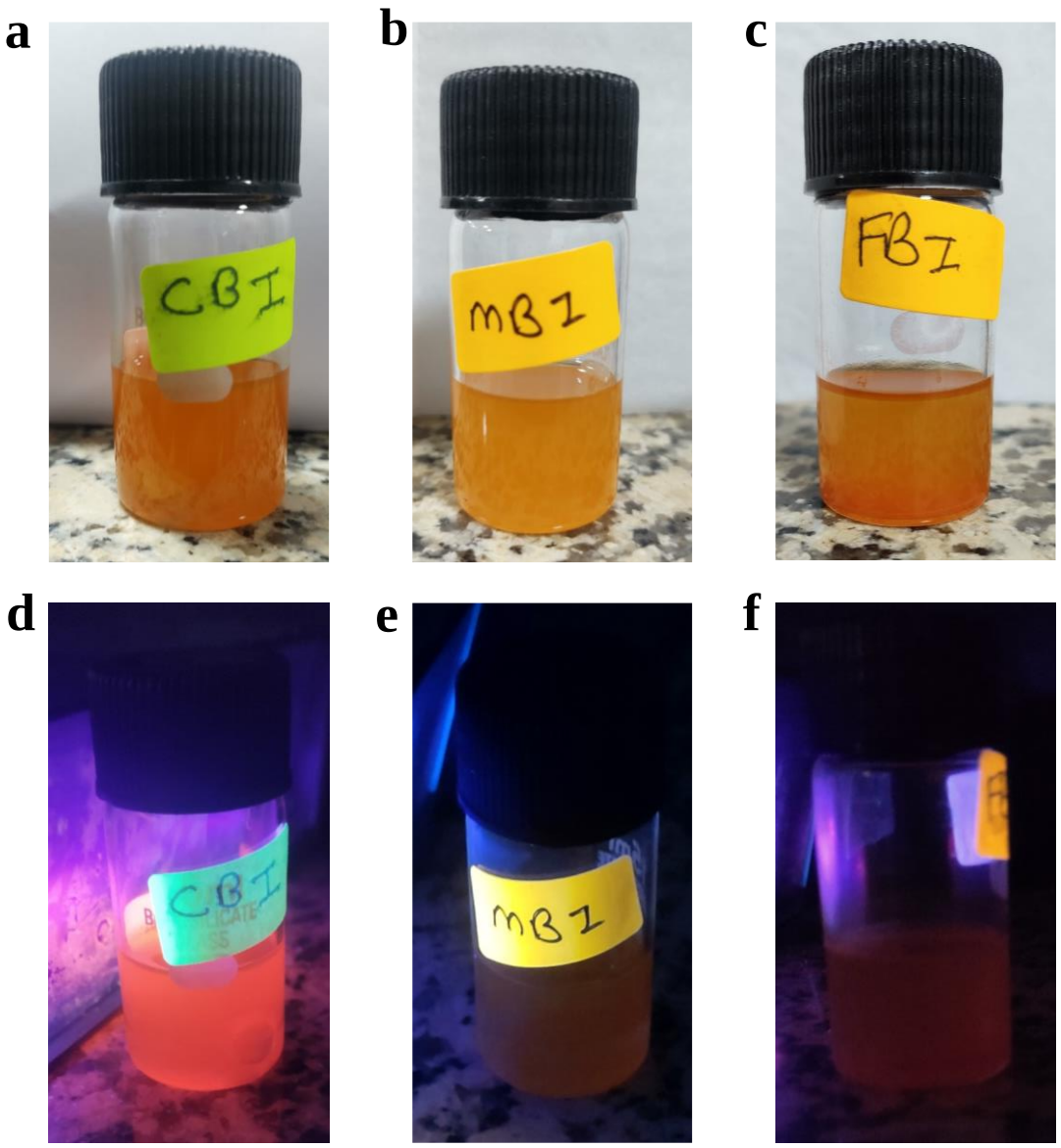

Figure S1. (a) Image of fabricated nanocrystals $Cs_3Bi_2I_9$, $MA_3Bi_2I_9$, and $FA_3Bi_2I_9$. (b) Image under UV light illumination.

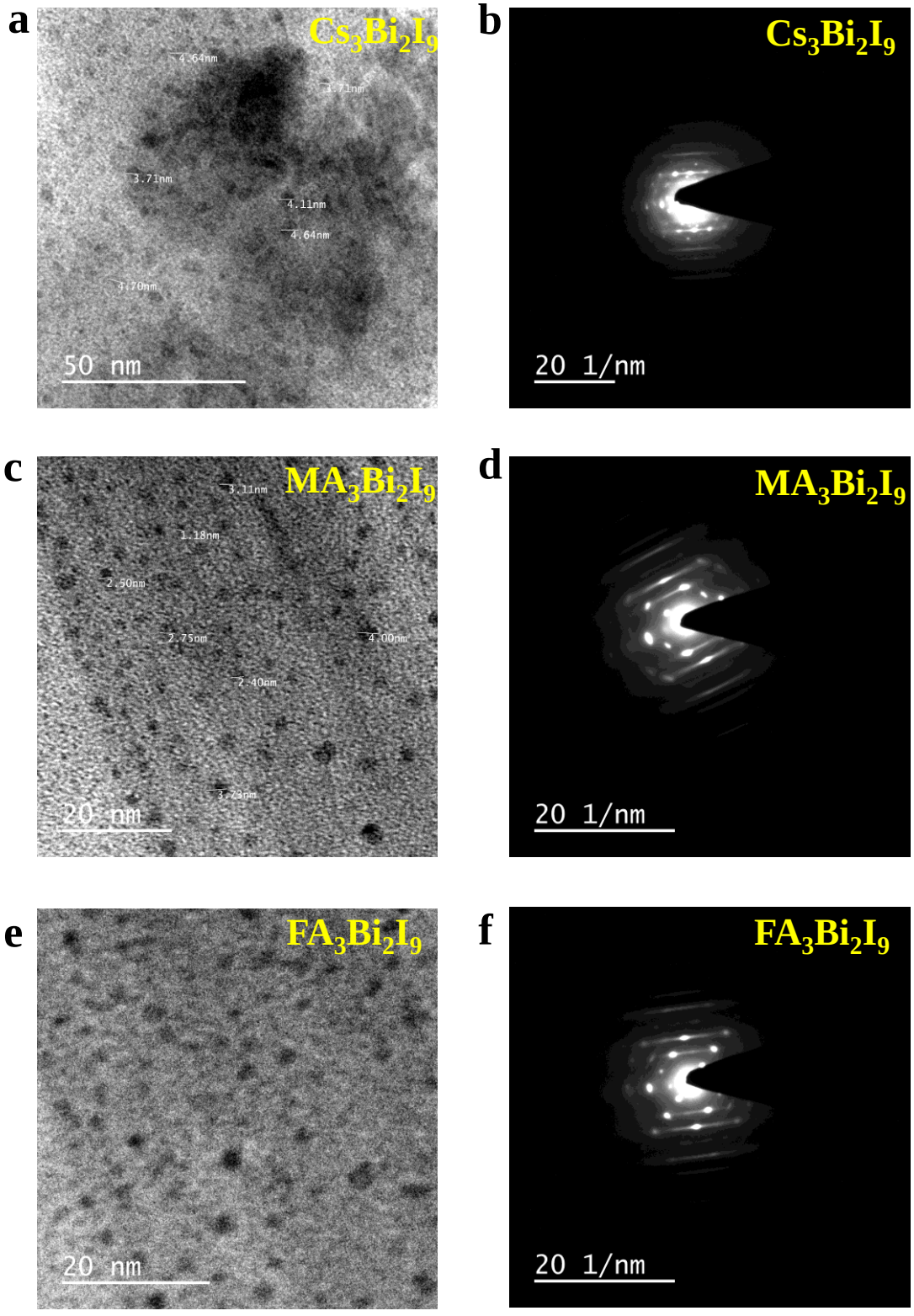

Figure S2. TEM image of the (a) $Cs_3Bi_2I_9$ NCs, (c) $MA_3Bi_2I_9$ NCs, (e) $MA_3Bi_2I_9$ NCs. Reciprocal pattern of (b) $Cs_3Bi_2I_9$ NCs, (d) $MA_3Bi_2I_9$ NCs, and (f) $FA_3Bi_2I_9$ NCs.

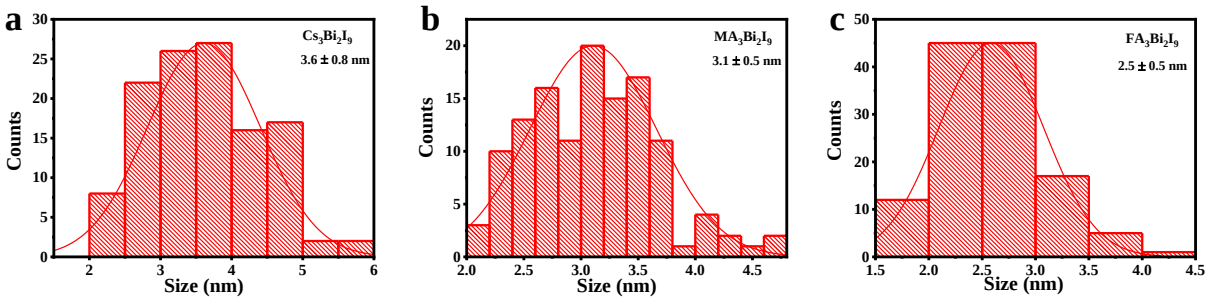

Figure S3. Size distribution of (a) $Cs_3Bi_2I_9$ NCs, (b) $MA_3Bi_2I_9$ NCs and (c) $FA_3Bi_2I_9$ NCs.

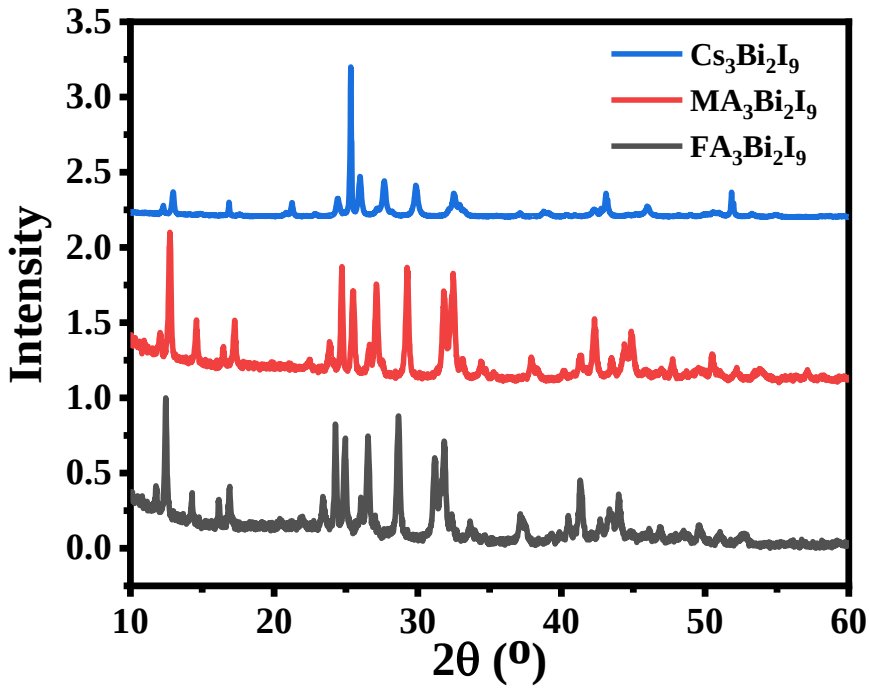

Figure S4. Powder XRD pattern of fabricated nanocrystal $Cs_3Bi_2I_9$, $MA_3Bi_2I_9$, and $FA_3Bi_2I_9$ powder.

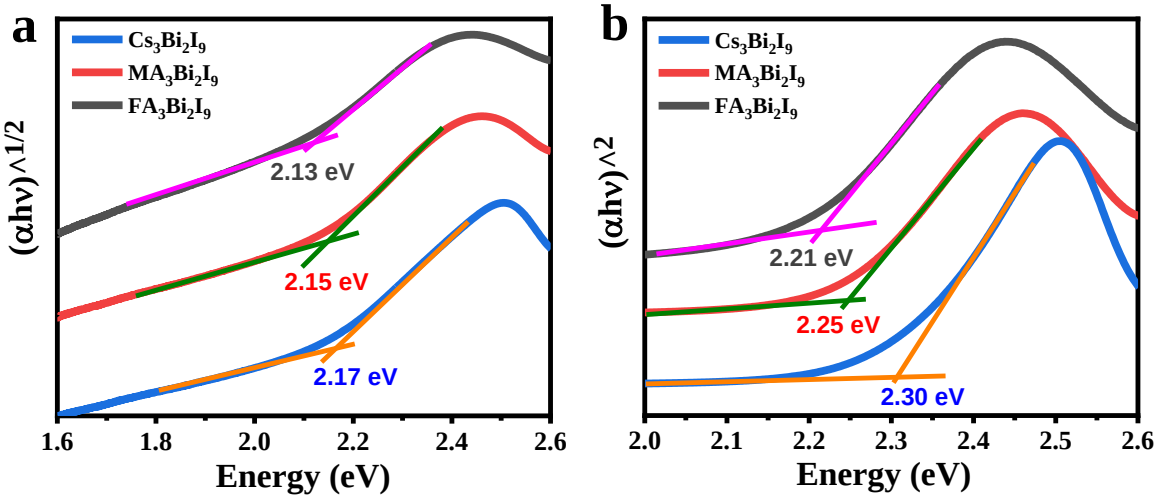

Figure S5. Calculated bandgap from tauc plot method. (a) indirect bandgap and (b) direct bandgap for all three systems.

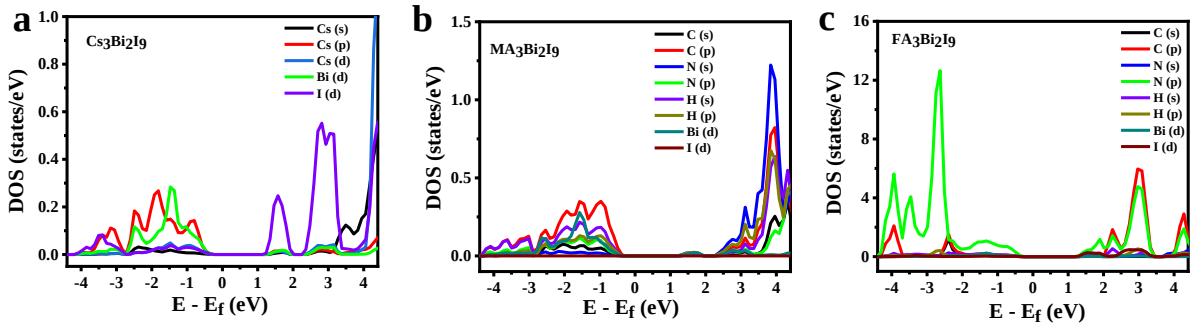

Figure S6. Atom-projected partial density of states (pDOS) for (a) $Cs_3Bi_2I_9$ (b) $MA_3Bi_2I_9$ and (c) $FA_3Bi_2I_9$.

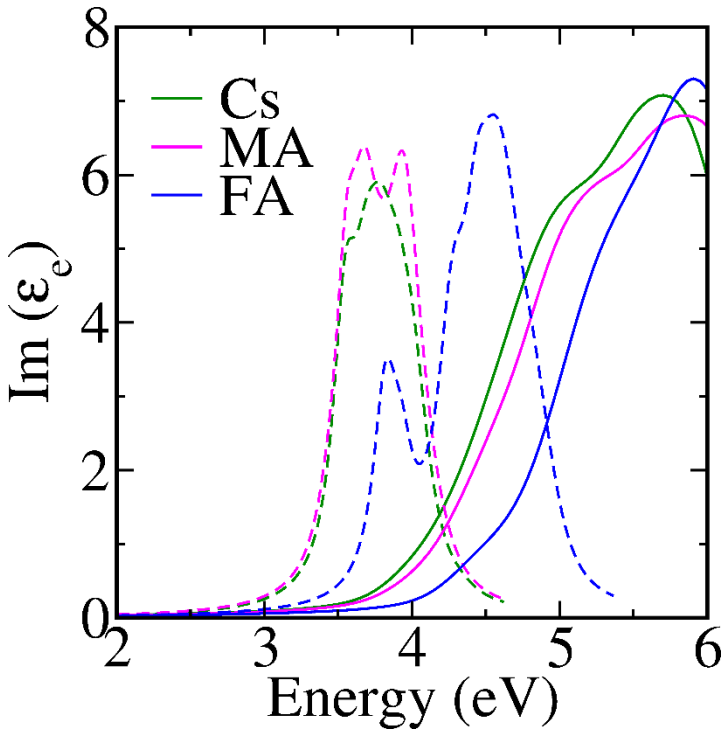

Figure S7. Electronic (solid) and optical spectra (dotted) of $Cs_3Bi_2I_9$, $MA_3Bi_2I_9$, and $FA_3Bi_2I_9$, estimated using G_0W_0 and mBSE on top of PBE exchange-correlation functional.

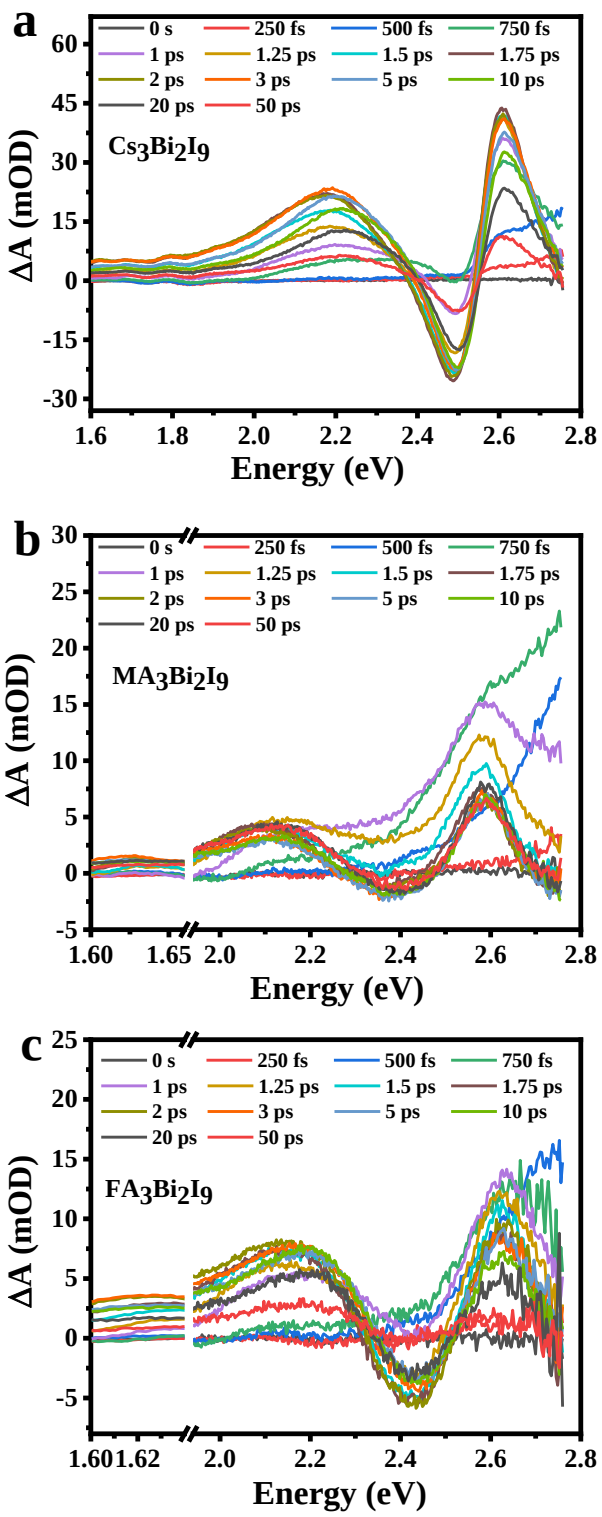

Figure S8. Femtosecond transient absorption (fs-TA) spectra in response to 350 nm optical excitation. Early time spectra up to 50 ps for (a) $Cs_3Bi_2I_9$, (b) $MA_3Bi_2I_9$, and (c) $FA_3Bi_2I_9$.

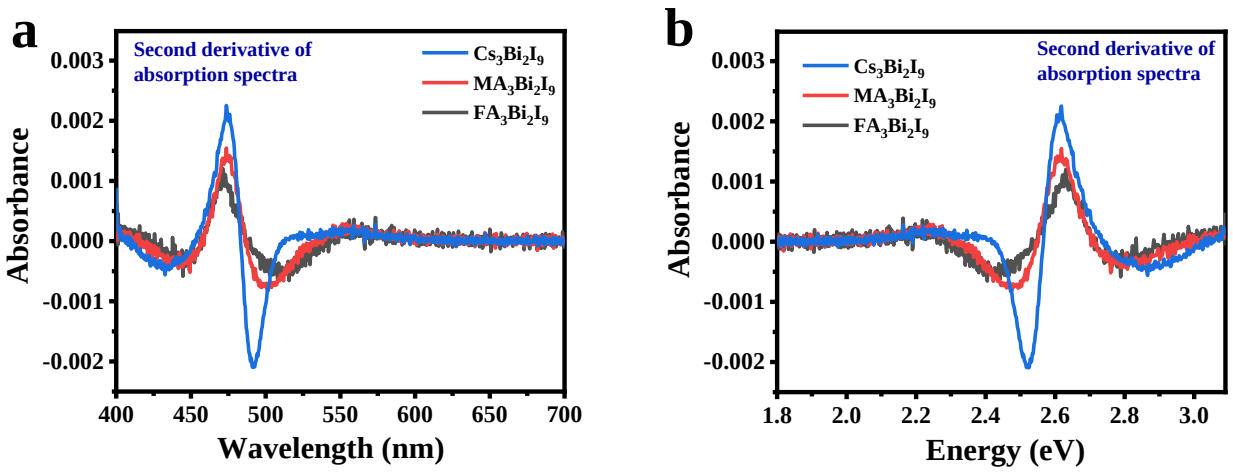

Figure S9. Smoothed second derivative of the steady-state absorption spectrum of $Cs_3Bi_2I_9$, $MA_3Bi_2I_9$, and $FA_3Bi_2I_9$ (a) wavelength scale and (b) energy scale.

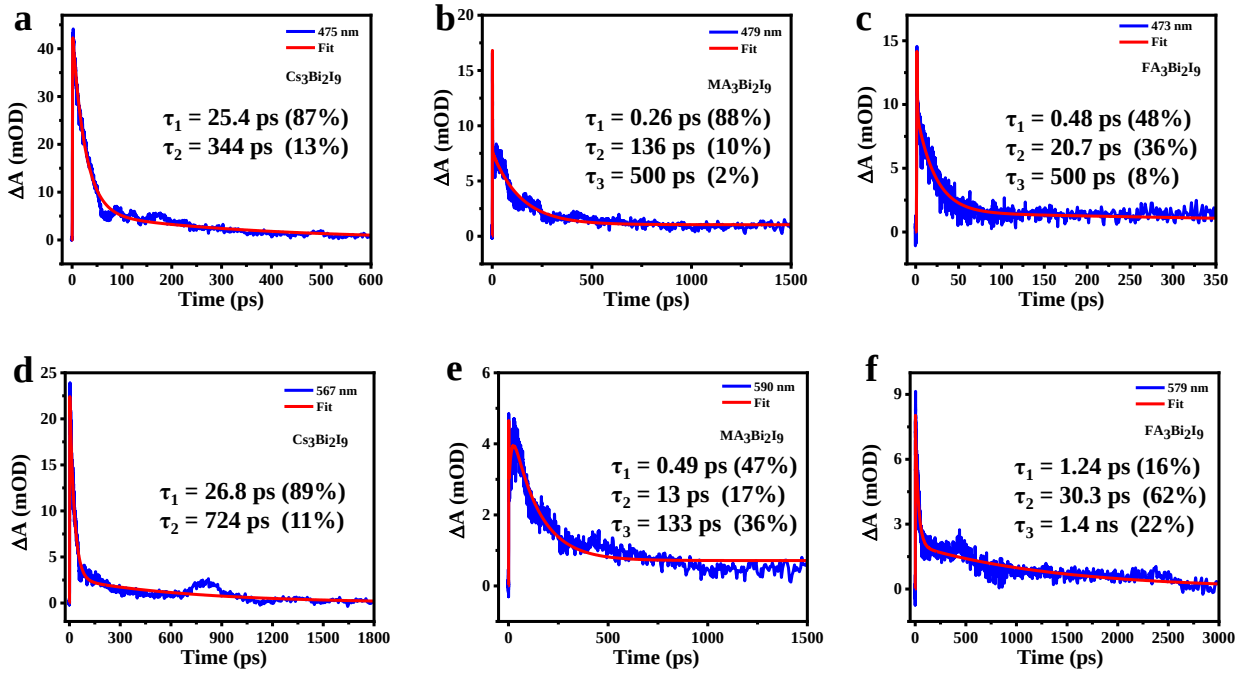

Figure S10. Kinetics at different probe wavelengths for all three systems. (a) $Cs_3Bi_2I_9$ at 475 nm, (b) $MA_3Bi_2I_9$ at 479 nm, (c) $FA_3Bi_2I_9$ at 473 nm, (d) $Cs_3Bi_2I_9$ at 567 nm, (b) $MA_3Bi_2I_9$ at 590 nm, (c) $FA_3Bi_2I_9$ at 579 nm.