Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Enhancing the Carrier Thermalization Time in Organometallic Perovskites by Halide Mixing

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Table S1: Averaged NA couplings (meV) and energy spacing $|\varepsilon_i - \varepsilon_j|$ (meV) between states (i and j) in the conduction and valence band for $MAPbI_3$.

i / j	NAC	$\lvert\varepsilon_i - \varepsilon_j\rvert$
VBM / VBM-1	8.7	151
VBM-1/ VBM-2	12.5	89
VBM-2 / VBM-3	21.4	60
VBM / VBM-2	2.6	241
VBM-1 / VBM-3	4.6	149
VBM-4 / VBM-5	20.4	58
VBM-6 / VBM-7	25.9	51
VBM-6 / VBM-8	8.7	101
VBM-7 / VBM-8	22.9	54
CBM / CBM+1	5.8	126
CBM+1 / CBM +2	7.3	134
CBM / CBM +2	2.5	260
CBM +2 / CBM +3	6.3	146
CBM+2 / CBM + 4	2.8	283
CBM+3 / CBM +4	6.6	137

Table S2: Averaged NA couplings (meV) and energy spacing $|\varepsilon_i - \varepsilon_j|$ (meV) between states (i and j) in the conduction and valence band for $MAPbI_3(Cl)$.

i / j	NAC	$\lvert\varepsilon_i - \varepsilon_j\rvert$
VBM / VBM-1	4.2	178
VBM-1/ VBM-2	15.4	76
VBM-2 / VBM-3	17.8	68
VBM / VBM-2	2.6	254
VBM-1 / VBM-3	5.6	144
VBM-4 / VBM-5	21.6	60
VBM-6 / VBM-7	14.2	81
VBM-6 / VBM-8	5.7	138
VBM-7 / VBM-8	20.3	57
CBM / CBM+1	4.7	171
CBM+1 / CBM +2	6.2	138
CBM / CBM +2	2	309
CBM +2 / CBM +3	5.4	150
CBM+2 / CBM + 4	2.1	286
CBM+3 / CBM +4	6.0	136

Table S3: Energy of CBM+n (VBM-n) relative to CBM (VBM) for the initial structures used in the nonadiabatic dynamics.

	MAPbI3	MAPbBr3	MAPbCl3	MAPbI3(Br)	MAPbI3(Cl)
CBM+1	0.10632	0.17255	0.09509	0.207919	0.207329
CBM+2	0.20984	0.31150	0.21372	0.289076	0.33763
CBM+3	0.33925	0.500498	0.36653	0.43325	0.484345
CBM+4	0.44510	0.601898	0.46593	0.527461	0.67451
CBM+5	0.61414	0.740627	0.62521	0.738535	0.88798
CBM+6	1.74798	1.562195	1.54266	1.30545	1.39471
CBM+7	1.86758	1.789367	1.72127	1.574698	1.710723
VBM-1	0.11567	0.177411	0.302022	0.166588	0.22196
VBM-2	0.20669	0.429995	0.432862	0.261419	0.315098
VBM-3	0.24988	0.4827654	0.549813	0.338413	0.389070
VBM-4	0.30358	0.573575	0.65664	0.409683	0.450781
VBM-5	0.35208	0.630696	0.710106	0.468546	0.507242
VBM-6	0.40305	0.682267	0.790257	0.527417	0.575930
VBM-7	0.45694	0.726131	0.867079	0.585351	0.659492
VBM-8	0.51059	0.768087	0.92432	0.623530	0.717617
VBM-9	0.57962	0.814564	0.97194	0.669781	0.783585
VBM-10	0.62609	0.861968	1.02207	0.728572	0.831394
VBM-11	0.67869	0.909950	1.07157	0.794469	0.8723842
VBM-12	0.73139	0.950748	1.109293	0.861516	0.9289179
VBM-13	0.78270	0.989159	1.15418	0.925059	0.9933742
VBM-14	0.87307	1.069757	1.24071	1.01477	1.1084115
VBM-15	0.87307	1.069757	1.24071	1.01477	1.1084115
VBM-16	0.93822	1.106887	1.28051	1.082313	1.162807
VBM-17	0.99533	1.143038	1.32680	1.179406	1.2294495

Figure S1: (a-e) Electron (hole) relaxation time (ps) from different excited states. **(f-j)** Population time (ps) of CBM01(VBM01) when initially populating different excited electron (hole) states

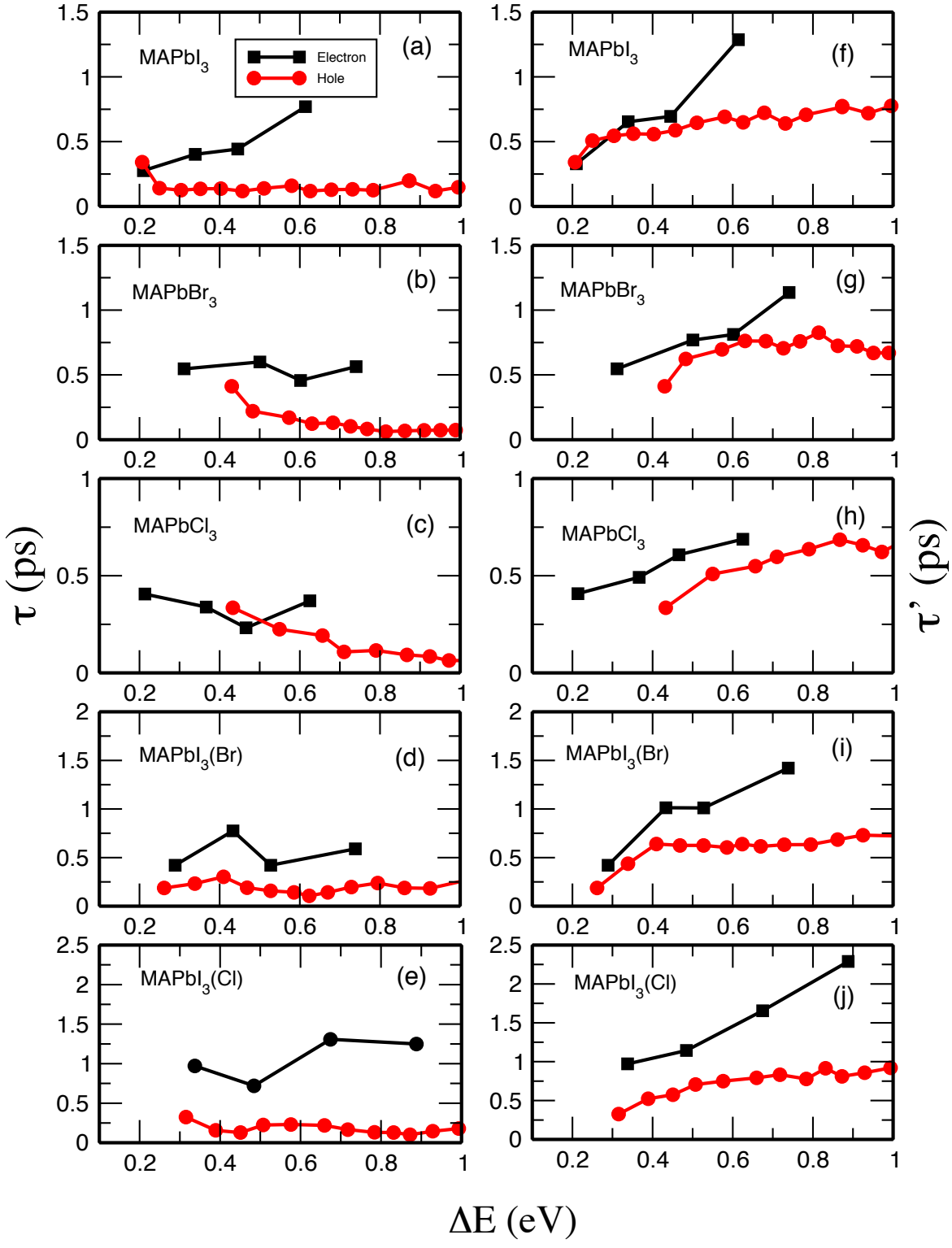

Figure S2: Influence spectra for the electron-phonon relaxation from different excited states in $MAPbI_3$, MAPbI(Cl) and $MAPbI_3$(Br).