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

Supporting Information

Ion Migration in Br-Doped $MAPbI_3$ and Its Inhibition Mechanisms Investigated Via Quantum Dynamics Simulations

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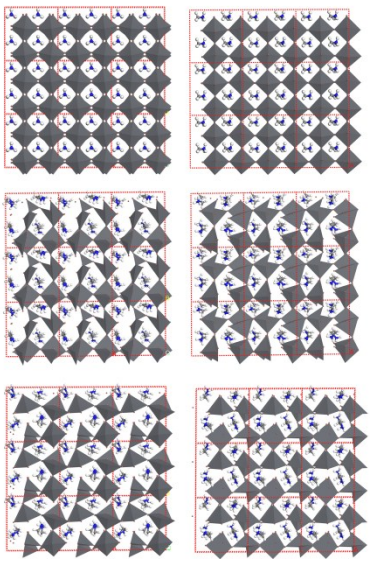

Fig. S1 Structures of the initial and equilibrium stage of $MAPbI_3$-450K from aob and cob view, respectively.

Table S1 The number of connections between two adjacent $[PbX_6]^{4-}$ octahedrons in $MAPb(I_{0.4}Br_{0.6})_3$

Time(ps)		Connection number	Total number	Ratio	Average ratio
Before migration	23ps	4	24	16.66%	24.16%
	39ps	8	24	33.33%	
	55ps	6	24	25.00%	
	71ps	4	24	16.66%	
	87ps	7	24	29.16%	
After migration	92ps	11	24	45.83%	33.33%
	119ps	6	24	25.00%	
	146ps	5	24	20.83%	
	173ps	10	24	41.66%	
	200ps	8	24	33.33%	

Table S2 The band gap values of $MAPb(I_{0.4}Br_{0.6})_3$

Time(ps)		Valence(eV)	Conduction(eV)	Band gap(eV)	Average (eV)
Before migration	23ps	-0.453	1.039	1.492	1.557
	39ps	-0.441	0.977	1.418	
	55ps	-0.434	1.326	1.760	
	71ps	-0.446	1.159	1.605	
	87ps	-0.436	1.074	1.510	
After migration	92ps	-0.438	0.979	1.417	1.450
	119ps	-0.453	1.114	1.567	
	146ps	-0.437	1.155	1.592	
	173ps	-0.465	0.851	1.316	
	200ps	-0.457	0.902	1.359	

Table S3 The number of connections between two adjacent $[PbX_6]^{4-}$ octahedrons in $Cs_{0.125}MA_{0.875}Pb(I_{0.4}Br_{0.6})_3$

Time(ps)	Connection number	Total number	Ratio	Average ratio
20ps	7	24	29.16%	32.08%
40ps	8	24	33.33%	
60ps	6	24	25.00%	
80ps	12	24	50.00%	
100ps	8	24	33.33%	
120ps	5	24	20.83%	
140ps	7	24	29.16%	
160ps	7	24	29.16%	
180ps	9	24	37.50%	
200ps	8	24	33.33%	

Table S4 The band gap values of $Cs_{0.125}MA_{0.875}Pb(I_{0.4}Br_{0.6})_3$

Time(ps)	Valence(eV)	Conduction(eV)	Band gap(eV)	Average (eV)
20ps	-0.462	0.967	1.429	1.562
40ps	-0.448	1.219	1.667	
60ps	-0.449	1.210	1.659	
80ps	-0.437	1.031	1.468	
100ps	-0.427	1.044	1.471	
120ps	-0.449	1.006	1.455	
140ps	-0.446	1.096	1.542	
160ps	-0.447	1.090	1.537	
180ps	-0.447	1.233	1.680	
200ps	-0.449	1.266	1.715	