

Supporting Information for

**Correlated Organic-Inorganic Motion Enhances Stability and
Charge Carrier Lifetime in Mixed Halide Perovskites**

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Atomic coordinates for pristine FAPbI₃

Pristine FAPbI₃

1.0000000000000000

12.7633421620310354 0.0000001219733521 -0.0000000335470497

0.0000001182129541 12.4366589113777088 -0.0000000870455447

-0.0000000347530897 -0.0000000859225700 12.4977923917214557

C N H Pb I

8 16 40 8 24

Direct

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0.7499999356487510 0.7608393821811998 0.2500000076724762

0.2500000772990797 0.2608393590699583 0.7500000014705072

0.7500000100569212 0.2608393591771004 0.7499999954847983

0.2500000568083398 0.7608393923908919 0.7500000012596766

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0.6586661494575191 0.2127873459888462 0.2500000032067766

0.3413338638166462 0.7127873342927097 0.2500000164660343

0.1586661004618961 0.7127873027909893 0.2499999839172351

0.8413339307587315 0.7127873141880116 0.2500000165350835

0.6586661537737980 0.7127873652011638 0.2499999921406878

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0.1586660790390402 0.2127872662084485 0.7499999943668781

0.8413338802745954 0.2127872907931229 0.7500000077648846

0.6586661214772070 0.2127873123547888 0.7499999941007650

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0.7499999880261563	0.3486917964401939	0.2500000017871423
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0.2499999960570816	0.8486917832852454	0.7499999979126114
0.4065260539390610	0.7602939175285921	0.7500000018295059
0.3510948437559394	0.6312009754343519	0.7499999888386374
0.1489051558546927	0.6312009704657723	0.7499999958841495
0.0934739672612526	0.7602939050645944	0.7499999884756040
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-0.0000000104035401	0.9828156197658334	-0.0000000005601340
0.5000000195645011	0.9828156383049778	0.0000000043132217
-0.0000000110564785	0.4828156232476932	0.5000000077519616
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-0.0000000079259519	0.9828156190030732	0.4999999987113936
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0.2499999994973081	0.4921003448289938	0.0000000041355082
0.0000000140276224	0.2312427490841786	-0.0000000259338976
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0.2499999877540537	0.9921003395485506	0.0000000047706841
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0.7499999952197903	0.4921003602044917	0.5000000170482896
0.4999999881007515	0.2312427283229705	0.5000000158580019
0.5000000171808846	0.4599756973470197	0.7499999980892842
0.2499999837186210	0.9921003345902111	0.5000000110782707
0.0000000028065516	0.7312427617599687	0.4999999934718656
0.0000000188392242	0.9599757724854500	0.7500000059748091
0.7499999954223249	0.9921003169215640	0.4999999904644739
0.5000000104915964	0.7312427474657167	0.4999999946747864
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Atomic coordinates for Br-doped FAPbI₃.

Br-doped FAPbI₃

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12.4828491456674211 -0.0000136965626238 0.0000000768145545

-0.0000136526951650 12.4633991760578606 0.0000000468921178

0.0000000845653015 0.0000000371098615 12.5545183041131754

C N H Pb I Br

8 16 40 8 20 4

Direct

0.2500054209125063 0.2612258679872021 0.2502966670784106

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0.2500053354549325 0.2612259038401333 0.7497033539836980

0.7499936532789678 0.2612257774020786 0.7497032750525860

0.2500041254907425 0.7612257369851182 0.7497033558725430

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