

## SUPPORTING INFORMATION

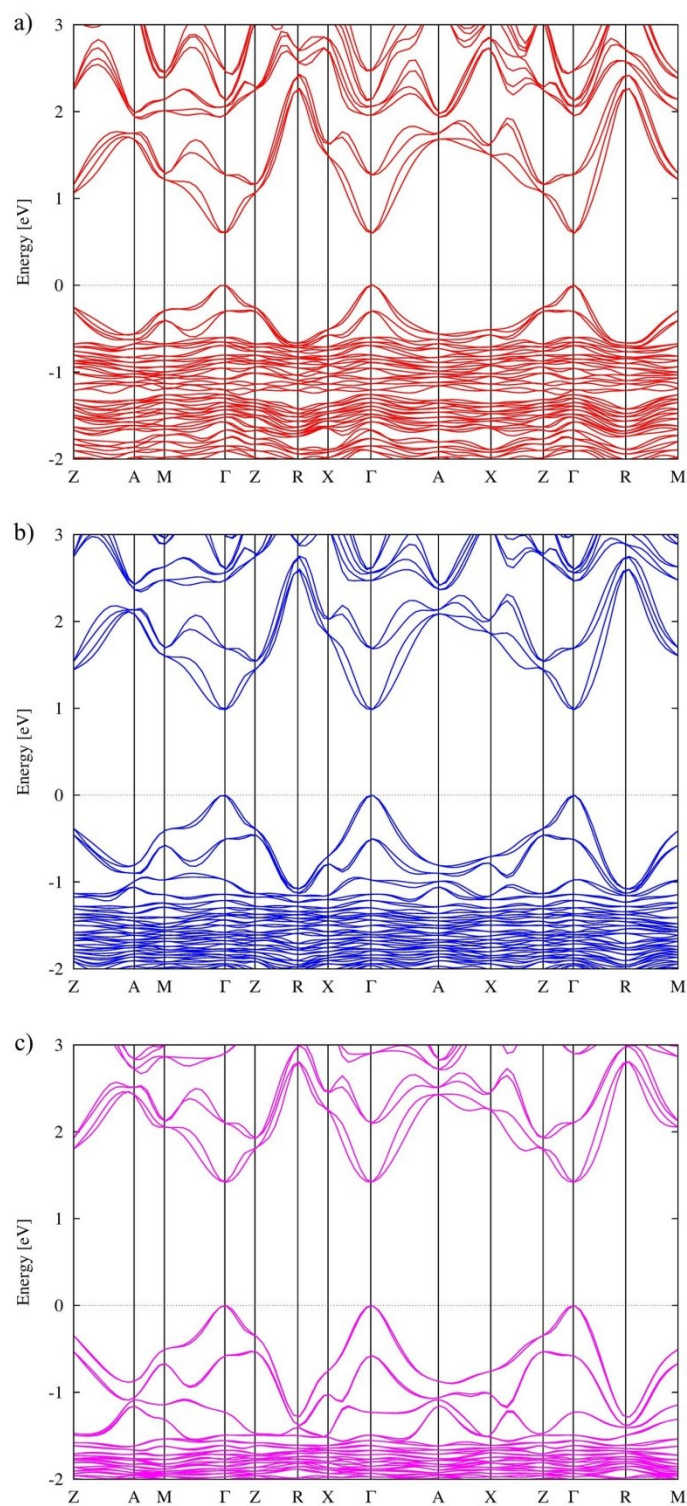
# Electronic and optical properties of $\text{MAPbX}_3$ perovskites ( $X = \text{I}, \text{Br}, \text{Cl}$ ): A unified DFT and GW theoretical analysis

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**Figure S1.** Band structure calculated for MAPbI<sub>3</sub> (a), MAPbBr<sub>3</sub> (b) and MAPbCl<sub>3</sub> (c) at the SOC-GGA level.

Table S1. Calculated band gap (eV) at different sampling of k-point for the MAPbI<sub>3</sub>.

k-point	SR-GGA	SOC-GGA
4x4x4	1.68	0.60
Γ	1.56	0.48

Optimized geometry structures

Cartesian coordinates MAPbI<sub>3</sub> with experimental cell parameters (Å):

Pb	1.053884348	-1.501188330	2.404986110
I	3.813256706	0.118025190	2.296272726
I	2.973537861	1.449113783	-3.552511737
Pb	1.156351973	-1.186067991	-3.896439625
I	-0.399339982	-4.014046437	-4.054910513
I	1.075637382	-1.571664114	-0.748716655
I	1.488045271	-1.390288161	5.595551692
I	-0.818794261	0.970250442	2.576730394
Pb	-3.347654341	2.829582136	2.484995990
I	-3.878527336	3.156204286	5.672472657
I	2.902031024	-4.181959406	2.332291985
I	3.906277901	-2.942350537	-3.663763581
I	-1.328149765	-3.570295657	2.891122301
I	-1.493420677	0.523031811	-3.927000860
Pb	-3.171232260	3.221045542	-3.873295424
I	-3.245995901	3.052576094	-0.674183949
C	1.015852294	2.353987139	5.643779913
N	1.017946281	3.835687709	5.450040759
H	1.357199243	1.875339231	4.718585038
H	1.693107119	2.113429995	6.473408793
H	-0.005201150	2.032064800	5.882532182
H	0.691917501	4.321501478	6.319875344
H	1.969208268	4.176315655	5.220111847
H	0.390007228	4.135921583	4.670696919
C	5.850893984	-1.242099357	5.783378101
N	4.930423800	-2.117936470	4.998927290
H	5.687312362	-1.434862123	6.850851191
H	6.886893254	-1.472474750	5.501714181
H	5.618762345	-0.195174382	5.548617061
H	5.060530185	-1.984708110	3.979219975
H	5.077061019	-3.132599115	5.209441365
H	3.927610528	-1.896966883	5.214413161
C	0.704198897	2.910765235	-0.491250991
N	1.843918696	3.722696868	-1.012642467
N	4.840372747	-0.660660987	-1.041409658
C	6.143793326	-1.262517420	-0.630683413
H	1.094952758	1.966269367	-0.092115133
H	0.204333732	3.473918807	0.307237121
H	0.005956169	2.713903508	-1.313957880
H	1.526552613	4.655277171	-1.349885290
H	2.543509884	3.900849453	-0.261367644
H	2.319348522	3.226533079	-1.800956531

H	5.945507321	-2.165235379	-0.038907660
H	6.712580475	-1.511638722	-1.534549294
H	6.696029572	-0.527734751	-0.030109307
H	4.974981712	0.254302113	-1.514263777
H	4.334763811	-1.286816472	-1.709541817
H	4.237498310	-0.488484754	-0.205424148

Cartesian coordinates MAPbBr<sub>3</sub> using experimental cell parameter (Å):

C	1.115309543	2.127107984	5.652300373
N	0.914918654	3.588134243	5.440166348
Br	1.503011402	-1.382830070	5.591635148
Pb	1.084478319	-1.455527253	2.624925412
Br	-1.156987043	-3.459125702	3.067782785
Br	3.695471737	0.003972496	2.514083568
Br	1.157275269	-1.502204460	-0.331345022
Pb	1.197467872	-1.146261002	-3.270924960
Br	-1.277609524	0.464688014	-3.176105161
Pb	-2.854925576	2.970928984	-3.229326785
Br	-2.896461207	2.780214962	-0.221208150
Pb	-3.068643413	2.582447973	2.714249904
Br	-3.467062302	2.895639024	5.697363397
Br	-0.701089356	0.817456678	2.845263635
Br	2.785123118	-3.938587931	2.626873122
Br	2.899144937	1.279159177	-2.852456920
Br	-0.237958971	-3.814975305	-3.391910830
Br	3.702513773	-2.883620013	-3.064195944
N	4.744480752	-2.002514957	5.063668670
C	5.632867252	-1.111321562	5.865225710
N	4.698170665	-0.704818862	-0.653583619
C	5.899697226	-1.402626505	-0.115707884
N	1.917009171	3.534407967	-0.575781169
C	0.777711306	2.746578571	-0.025179089
H	1.486128849	1.685707587	4.721465248
H	1.843252677	1.990427737	6.461157678
H	0.153453355	1.675589671	5.923006000
H	0.613672999	4.053986975	6.329177934
H	1.784406473	4.038988708	5.105199821
H	0.192167942	3.795221062	4.712049182
H	5.506796371	-1.355224872	6.925995128
H	6.673351258	-1.267529310	5.554441740
H	5.340073180	-0.068755829	5.684517615
H	4.841782832	-1.816515943	4.048963419
H	4.942209714	-3.013417750	5.230806869
H	3.737588696	-1.832407828	5.301916328
H	1.156395747	1.786803815	0.345584068
H	0.317721487	3.309481252	0.795817863
H	0.050422081	2.579777135	-0.827659374
H	1.616651071	4.491790024	-0.855758379
H	2.660040396	3.658371188	0.138664554
H	2.327088624	3.045231617	-1.402065524
H	5.578465077	-2.318172357	0.395908282
H	6.562979741	-1.646044414	-0.952686769
H	6.410040832	-0.732411069	0.587445432
H	4.949614285	0.201494070	-1.090239256
H	4.229894008	-1.291378343	-1.381867220

H 4.023709702 -0.500046577 0.112885823

Cartesian coordinates MAPbCl<sub>3</sub> with experimental cell parameters (Å):

Pb	0.937020143	-1.381620552	2.098848798
Cl	3.211929739	0.317599239	1.844273817
Cl	2.699872755	1.301845443	-3.305788426
Pb	0.964431461	-1.008900183	-3.532207636
Cl	-0.489754419	-3.511397613	-3.633088932
Cl	1.034885395	-1.534215680	-0.759835038
Cl	1.409893953	-1.285797523	4.938867114
Cl	-1.132155996	0.537298685	2.399452065
Pb	-3.080944681	2.580388321	2.231991058
Cl	-3.279652103	3.073405815	5.085611211
Cl	2.703232904	-3.640473759	2.225540867
Cl	3.347432086	-2.614462807	-3.350845770
Cl	-1.134693736	-3.338622116	2.539171237
Cl	-1.378510211	0.684905164	-3.215713026
Pb	-2.973784309	3.022014726	-3.468219920
Cl	-3.189002236	2.822985615	-0.579682726
C	1.011249439	2.100007146	4.846637634
N	0.768103727	3.569701583	4.900244063
H	1.391401901	1.843649875	3.850768134
H	1.746556583	1.834665268	5.616021108
H	0.062189194	1.581313485	5.022904990
H	0.406354704	3.873014073	5.836799757
H	1.632027238	4.102254012	4.702229080
H	0.072765972	3.875031075	4.176030363
C	5.346104178	-0.892597492	5.376031513
N	4.556882827	-1.662165641	4.369176663
H	5.057137431	-1.239196765	6.374216016
H	6.413413086	-1.069268376	5.196888416
H	5.117813950	0.175515396	5.266776856
H	4.771458453	-1.350482932	3.407072251
H	4.746496105	-2.685664408	4.434941757
H	3.528634541	-1.528108529	4.524757283
C	0.602056880	2.494670338	-0.198488995
N	1.599120434	3.253212641	-1.010040233
N	4.494548212	-0.640988937	-1.050826182
C	5.452038014	-1.591220629	-0.416658882
H	1.019923491	1.507847799	0.035942296
H	0.405831256	3.047246714	0.727770443
H	-0.320919033	2.386376409	-0.780236952
H	1.299347740	4.237973746	-1.174416380
H	2.528500760	3.284664511	-0.540992123
H	1.765769882	2.779408882	-1.926239918
H	4.889643075	-2.438266266	-0.008625119
H	6.159405961	-1.941750558	-1.177483464
H	5.987760207	-1.066352016	0.382960466
H	5.004402403	0.128660156	-1.526288120
H	3.934931011	-1.136283995	-1.781604973
H	3.860276085	-0.233082640	-0.332648827