Supplemental Material: Impact of symmetry breaking and spin-orbit coupling on the band gap of halide perovskites

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Main results for the calculated halide pervskites

Table SM1: Calculated band gaps and lattice parameters for all calculated halide perovskites. The lattice parameter was optimized with the PBE exchange and correlation functional and shown for the monomorphous (Pm-3m) cubic perovskite. We also show the band gap calculated with the HSE06 exchange and correlation functional for monorphous and polymorphous structural configuration. Only systems based on Cs at the A site have the band gap calculated with the addition of spin-orbit coupling (SOC).

System	Lattice parameter Mono. (Å)	Band gap Mono. (eV)	Band gap Mono. +SOC (eV)	Band gap Poly. (eV)	Band gap Poly. +SOC (eV)
CsAlCl3	5.18	0.00	0.00	1.65	1.65
CsBaBr3	6.35	5.12	5.02	5.35	5.26
CsBaCl3	6.05	5.91	5.88	6.17	6.15
CsBaF3	5.11	7.08	6.93	7.50	7.41
CsBaI3	6.78	4.46	4.24	4.79	4.55
CsBeCl3	4.85	3.42	3.38	5.48	5.47
CsBeF3	4.04	7.26	6.95	9.21	9.20
CsCaBr3	5.77	5.55	5.44	5.62	5.53
CsCaCl3	5.47	6.66	6.63	6.66	6.63
CsCaF3	4.58	8.97	8.92	8.97	8.92
CsCaI3	6.23	4.72	4.49	4.82	4.65
CsCdBr3	5.62	1.85	1.67	2.10	1.95
CsCdCl3	5.33	3.04	3.03	3.04	3.03
CsCdF3	4.56	5.28	5.27	5.28	5.27
CsCdI3	6.05	0.53	0.21	2.38	2.16
CsGaBr3	5.51	0.00	0.00	0.71	0.71
CsGaCl3	5.22	0.00	0.00	0.97	0.97
CsGeBr3	5.60	1.13	1.02	1.56	1.45
CsGeCl3	5.34	1.65	1.46	2.14	2.03
CsGeF3	4.55	3.03	2.86	4.51	4.47
CsGeI3	6.00	1.00	0.71	1.51	1.35
CsHgBr3	5.67	0.00	0.00	1.95	1.92

CsHgCl3	5.40	0.51	0.47	2.22	2.19
CsHgF3	4.67	2.43	2.32	2.49	2.39
CsHgI3	6.09	0.00	0.00	2.09	1.95
CsInBr3	5.76	0.00	0.00	0.39	0.39
CsInCl3	5.48	0.00	0.00	2.26	2.26
CsMgBr3	5.45	3.65	3.53	3.65	3.54
CsMgCl3	5.13	5.31	5.28	5.31	5.29
CsMgF3	4.25	8.82	8.65	8.83	8.67
CsMgI3	5.91	2.03	1.78	2.27	2.05
CsPbBr3	5.99	2.41	1.25	2.87	1.79
CsPbCl3	5.72	2.92	1.78	3.35	2.27
CsPbF3	4.86	3.97	2.97	4.19	3.20
CsPbI3	6.39	2.00	0.77	2.46	1.35
CsSnBr3	5.89	1.10	0.70	1.81	1.53
CsSnCl3	5.62	1.56	1.17	2.38	2.13
CsSnF3	4.78	2.56	2.25	4.15	4.05
CsSnI3	6.27	0.81	0.37	1.50	1.18
CsSrBr3	6.03	5.32	5.21	5.51	5.43
CsSrCl3	5.72	6.27	6.24	6.47	6.47
CsSrF3	4.83	8.20	8.18	8.24	8.23
CsSrI3	6.47	4.58	4.36	4.76	4.57
CsTlBr3	5.89	0.00	0.00	0.20	0.20
CsTlF3	4.79	0.00	0.00	2.64	2.63
CsZnBr3	5.38	1.23	1.09	3.22	3.15
CsZnCl3	5.08	2.72	2.68	4.35	4.34
CsZnF3	4.29	5.96	5.95	6.00	6.00
CsZnI3	5.83	0.00	0.00	3.05	2.87
AgGeCl3	5.17	0.00		3.64	
AgMgF3	3.98	4.22		4.06	
AgSnCl3	5.44	0.00		3.64	
AgZnF3	4.07	3.87		3.50	
BaLiBr3	5.22	4.60		5.65	
BaLiCl3	4.91	5.56		6.50	
BaLiF3	4.05	8.66		8.65	
CaAgCl3	5.31	2.92		3.87	
CaInI3	6.13	3.25		3.17	
CdAgCl3	5.18	2.74		2.80	
CdAgF3	4.42	2.98		3.06	
CdInI3	5.91	0.65		1.01	
HgBiCl3	5.46	0.90		1.43	

InCaBr3	5.69	4.14	4.19
InCaCl3	5.39	4.76	4.56
InCaF3	4.50	4.60	4.11
InCdBr3	5.53	1.95	2.29
InCdCl3	5.25	3.08	2.41
InCdF3	4.48	4.27	3.31
InGaCl3	5.12	0.00	2.44
InGeBr3	5.51	0.97	2.55
InGeCl3	5.25	1.43	3.22
InGeI3	5.88	0.74	2.09
InHgI3	5.98	0.00	1.94
InMgCl3	5.01	4.47	4.36
InMgF3	4.11	3.85	3.85
InPbBr3	5.93	2.23	3.18
InPbCl3	5.67	2.44	3.72
InPbF3	4.81	2.54	3.80
InPbI3	6.32	1.90	2.58
InSnBr3	5.82	0.93	2.70
InSnCl3	5.56	1.19	3.35
InSnF3	4.70	1.18	3.35
InSnI3	6.19	0.63	1.92
InZnF3	4.18	3.75	3.68
KBaCl3	6.03	5.42	5.91
KBeF3	3.74	9.97	10.49
KCaBr3	5.72	5.04	5.51
KCaCl3	5.40	6.04	6.53
KCaF3	4.48	8.18	8.45
KCdBr3	5.56	1.91	2.62
KCdCl3	5.26	3.14	3.58
KCdF3	4.47	5.07	5.18
KCdI3	6.00	0.55	2.92
KGaBr3	5.45	0.00	1.46
KGaCl3	5.13	0.00	2.36
KGaF3	4.28	0.00	3.25
KGeBr3	5.54	1.08	2.66
KGeCl3	5.26	1.42	3.31
KGeF3	4.45	2.95	5.34
KGeI3	5.93	0.86	2.13
KHgBr3	5.63	0.00	2.62
KHgCl3	5.34	0.52	3.09

KHgF3	4.60	2.30	2.97
KHgI3	6.04	0.00	2.53
KInBr3	5.71	0.00	1.01
KInCl3	5.42	0.00	1.98
KMgBr3	5.36	3.82	4.23
KMgCl3	5.02	5.63	5.74
KMgF3	4.05	9.24	9.25
KMgI3	5.84	2.07	3.02
KPbBr3	5.95	2.36	3.33
KPbCl3	5.68	2.88	3.90
KPbF3	4.81	3.95	4.83
KPbI3	6.36	1.96	2.81
KSnBr3	5.84	1.00	2.69
KSnCl3	5.57	1.43	3.51
KSnF3	4.71	2.60	4.55
KSnI3	6.24	0.73	2.06
KSrCl3	5.69	5.71	6.19
KSrF3	4.77	7.43	7.78
KTlF3	4.66	0.00	3.22
KZnBr3	5.29	1.33	3.90
KZnCl3	4.97	2.96	4.75
KZnF3	4.13	6.08	6.09
LiCdF3	4.42	4.46	5.26
LiGaBr3	5.36	0.00	2.83
LiGaI3	5.80	0.00	1.64
LiGeCl3	4.67	1.99	4.02
LiZnF3	4.03	5.44	6.12
MgAgCl3	4.91	3.11	4.41
MgInBr3	5.33	0.00	0.48
MgTlBr3	5.77	0.00	4.12
NaCaCl3	5.36	5.05	6.19
NaCaF3	4.43	7.00	7.64
NaCdCl3	5.22	4.52	4.05
NaCdF3	4.43	4.52	5.07
NaGeCl3	5.22	1.27	4.54
NaHgCl3	5.31	0.53	3.51
NaHgF3	4.57	2.11	3.47
NaMgCl3	4.96	5.40	5.67
NaMgF3	3.94	8.11	8.64
NaPbCl3	5.03	2.84	4.11

NaPbF3	4.79	2.96	4.78
NaSnBr3	5.33	1.70	3.31
NaSnCl3	5.02	2.58	4.08
NaSnF3	4.67	1.75	4.37
NaZnCl3	4.91	3.06	5.09
NaZnF3	4.05	5.53	5.86
PbLiF3	3.90	5.31	5.66
RbBaCl3	6.04	5.59	5.94
RbBaF3	5.12	6.56	7.15
RbBaI3	6.78	4.18	4.69
RbBeF3	3.86	9.19	9.73
RbCaBr3	5.74	5.22	5.58
RbCaCl3	5.43	6.26	6.51
RbCaF3	4.52	8.45	8.52
RbCaI3	6.20	4.41	4.80
RbCdBr3	5.58	1.88	2.38
RbCdCl3	5.29	3.10	3.39
RbCdF3	4.50	5.15	5.19
RbCdI3	6.02	0.54	2.57
RbGaBr3	5.46	0.00	0.61
RbGaCl3	5.16	0.00	1.35
RbGeBr3	5.56	1.12	2.31
RbGeCl3	5.29	1.51	2.84
RbGeF3	4.48	2.98	5.09
RbGeI3	5.95	0.90	1.89
RbHgBr3	5.65	0.00	2.59
RbHgCl3	5.36	0.52	2.82
RbHgF3	4.63	2.35	2.72
RbHgI3	6.06	0.00	2.42
RbInBr3	5.73	0.00	1.14
RbInCl3	5.45	0.00	1.54
RbMgBr3	5.39	3.75	3.93
RbMgCl3	5.06	5.50	5.51
RbMgF3	4.12	9.23	9.24
RbMgI3	5.87	2.05	2.68
RbPbBr3	5.97	2.38	3.08
RbPbCl3	5.70	2.90	3.63
RbPbF3	4.93	2.31	4.78
RbPbI3	6.37	1.98	2.66
RbSnBr3	5.86	1.03	2.34

RbSnF3	4.74	2.63	4.48
RbSnI3	6.25	0.77	1.91
RbSrBr3	6.01	5.01	5.40
RbSrCl3	5.70	5.90	6.22
RbSrF3	4.79	7.69	7.95
RbSrI3	6.50	1.83	4.63
RbTlBr3	5.86	0.00	0.29
RbTlCl3	5.58	0.00	0.90
RbTlF3	4.68	0.00	2.77
RbZnBr3	5.33	1.29	3.87
RbZnCl3	5.01	2.86	4.53
SnLiF3	3.88	4.23	4.50
SnTlF3	4.70	1.27	3.71
SrInBr3	5.95	4.02	3.57
SrLiF3	3.88	9.40	9.95
SrTlCl3	5.70	0.00	4.95
TlCaBr3	5.69	4.29	4.90
TlCaCl3	5.39	5.12	5.41
TlCaF3	4.50	5.88	5.48
TlCaI3	6.14	3.40	4.28
TlCdBr3	5.53	1.94	2.99
TlCdCl3	5.25	3.19	3.34
TlCdF3	4.48	5.52	4.97
TlCdI3	5.95	0.60	2.85
TlGeBr3	5.51	1.03	2.48
TlGeCl3	5.25	1.41	3.14
TlGeF3	4.46	2.28	4.08
TlGeI3	5.89	0.76	2.10
TlHgBr3	5.60	0.00	2.75
TlHgCl3	5.33	0.54	3.13
TlHgF3	4.60	3.17	3.57
TlHgI3	5.99	0.00	2.48
TlInCl3	5.54	0.00	1.96
TlMgCl3	5.02	5.41	5.41
TlMgF3	4.11	5.42	5.42
TlPbBr3	5.93	2.33	3.21
TlPbCl3	5.67	2.60	3.75
TlPbF3	4.81	2.66	4.33
TlPbI3	6.32	1.91	2.76
TlSnBr3	5.82	0.95	2.55

TlSnI3	6.20	0.66	1.97
TlSrF3	4.77	5.93	5.56
TlZnBr3	5.26	1.39	3.54
TlZnCl3	4.96	2.97	4.12
TlZnF3	4.18	5.25	5.25
ZnAgCl3	4.87	2.92	3.47
ZnInCl3	4.96	2.09	3.36