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Supplementary Information: Stable hybrid organic-inorganic halide perovskites for photovoltaics from *ab-initio* high-throughput calculations

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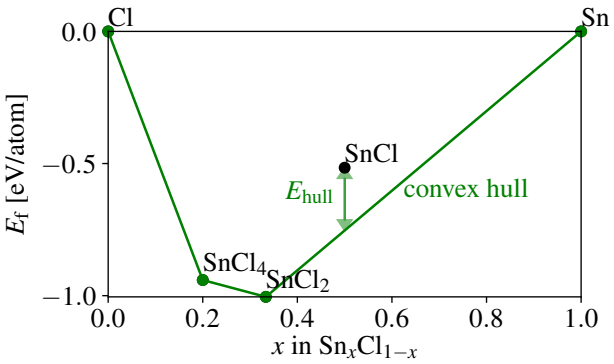

Fig. ESI-1 (Color online) Formation energy E_f (in units of eV/atom) as a function of composition for the system Sn-Cl. Stable compounds (those on the convex hull) are connected by a green line. For the sake of readability, many unstable or metastable phases are omitted.

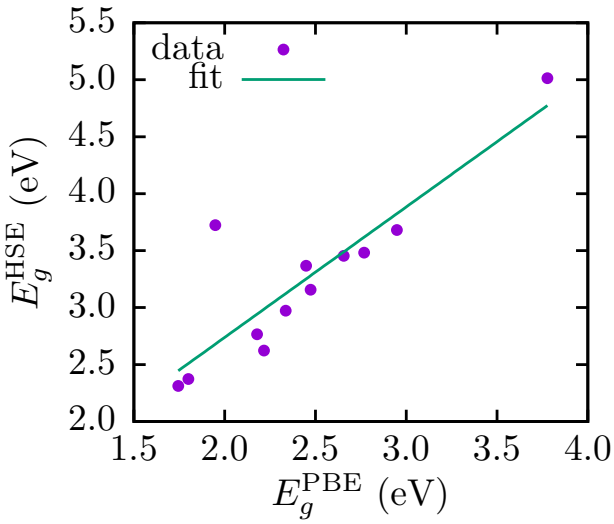

Fig. ESI-2 (Color online) Linear fit between PBE and HSE gaps for lead compounds, used to estimate HSE gaps in cases where we did not perform the actual HSE calculation.

Convex hull of stability

A convex hull is shown in Fig. ESI-1 for the example of the binary phase diagram Sn–Cl. If a compound is stable with respect to decomposition, it lies by definition on the convex hull; otherwise it lies above the hull. As SnCl lies above the hull, it is unstable, in this case with respect to decomposition into $SnCl_2$ and Sn.

Lead halides

We fit calculated HSE gaps for lead halides by $E_g^{\mathrm{HSE}} = a \cdot E_g^{\mathrm{PBE}} + b + \Delta E_{\mathrm{SOC}}$, where E_g^{HSE} is the calculated direct HSE gap without considering spin-orbit coupling (SOC), E_g^{PBE} is the calculated PBE gap, also without considering SOC, ΔE_{SOC} is the gap reduction from spin-orbit coupling calculated on PBE level, and a and b are fit parameters. The resulting fit parameters are $a = 1.14538$ and $b = 0.447468$. ΔE_{SOC} is set to -1.0 eV. The fit is then used to estimate direct gaps of metastable lead halides, for which we did not perform a HSE calculation.

All data

Tables ESI-1 to ESI-5 contain the calculation results for all stable compounds.

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Table ESI-1 Calculated properties of ABX_3 compounds: distance from the convex hull E_{hull} in eV/atom, magnetic moment μ of the unit cell in units of the Bohr magneton, fundamental and direct band gaps from PBE and HSE06 functionals (including SOC), effective mass m^* in units of the electron mass, and formation energies E_{f} in eV/atom

			PBE gap		HSE gap					
composition	E_{hull}	μ/μ_B	fund. (SOC)	direct (SOC)	fund.	direct	m^*	m_e^*	m_h^*	E_{f}
H_3SInCl_3-1D-W	0.000	0.0	2.54(-0.00)	2.64 (-0.00)			7.11	7.14	>1000	-0.565
$GCdBr_3-1D-W\bullet$	0.000	0.0	3.44(-0.14)	3.44 (-0.14)			0.64	0.67	13.88	-0.507
$GCdI_3-1D-W$	0.000	0.0	2.35(-0.25)	2.35 (-0.25)			3.43	4.07	21.76	-0.393
$NH_4GeCl_3-3D-OR$	0.000	0.0	2.88(-0.04)	2.88 (-0.04)			0.50	1.38	0.79	-0.693
$GCdCl_3-1D-W$	0.000	0.0	4.13(-0.00)	4.13 (-0.00)			0.78	0.81	28.03	-0.583
NH_4GeF_3-1D-W	0.000	0.0	4.05(-0.00)	4.06 (-0.00)			43.22	59.31	159.26	-1.334
NH_4CaCl_3-1D-R	0.000	0.0	5.12(-0.01)	5.12 (-0.01)			0.42	0.44	11.27	-1.211
$H_3SAuBr_3-3D-OR$	0.000	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.211
$GCaCl_3-1D-W$	0.000	0.0	5.06(-0.00)	5.06 (-0.00)			0.99	1.01	88.94	-0.858
H_3SPbBr_3-1D-R	0.000	0.0	2.51(-0.49)	2.59 (-0.50)			8.45	11.27	33.82	-0.499
$MPCaI_3-1D-W$	0.000	0.0	3.33(-0.20)	3.33 (-0.20)			1.27	1.32	31.50	-0.534
NH_4CoCl_3-1D-W	0.000	12.0	0.00(-0.01)	0.00 (-0.01)	3.60	3.61	55.42	>1000	55.42	-0.590
$GPbBr_3-1D-W$	0.000	0.0	3.13(-0.60)	3.18 (-0.60)			2.59	2.82	31.94	-0.515
NH_4MnCl_3-1D-R	0.000	20.0	1.99(-0.00)	2.03 (-0.00)			113.91	148.99	483.71	-0.760
$GSrBr_3-1D-W$	0.000	0.0	4.54(-0.13)	4.54 (-0.12)			0.60	0.62	25.57	-0.761
$MPBeCl_3-1D-W$	0.000	0.0	5.05(-0.01)	5.07 (-0.01)			8.97	9.29	259.89	-0.561
$GSrI_3-1D-W$	0.000	0.0	3.80(-0.29)	3.81 (-0.29)			3.40	7.22	6.44	-0.636
H_3SSnBr_3-1D-R	0.000	0.0	2.35(-0.08)	2.54 (-0.08)			7.30	14.51	14.70	-0.439
$GCaI_3-1D-W$	0.000	0.0	3.65(-0.27)	3.65 (-0.27)			27.29	160.62	32.88	-0.624
NH_4PbBr_3-1D-R	0.000	0.0	2.39(-0.46)	2.47 (-0.47)			2.09	3.76	4.70	-0.686
$GSnBr_3-1D-W$	0.000	0.0	3.23(-0.07)	3.26 (-0.07)			2.54	3.07	14.90	-0.484
$MPInCl_3-1D-W$	0.000	0.0	2.33(-0.00)	2.53 (-0.00)			1.58	1.58	>1000	-0.448
$GPbI_3-1D-W$	0.000	0.0	2.59(-0.68)	2.66 (-0.66)			0.78	0.94	4.70	-0.416
$MPSnBr_3-3D-OR$	0.000	0.0	1.63(-0.19)	1.63 (-0.19)	2.19	2.19	0.22	0.58	0.35	-0.373
NH_4HgCl_3-1D-R	0.000	0.0	2.35(-0.02)	2.50 (-0.01)			0.55	0.56	31.36	-0.605
$MPSrI_3$	0.000	0.0	3.41(-0.18)	3.51 (-0.28)			0.42	0.46	5.15	-0.549
H_3SSnI_3-1D-R	0.000	0.0	1.98(-0.18)	2.05 (-0.19)			4.66	13.89	7.02	-0.274
$GSnCl_3-1D-W$	0.000	0.0	3.73(-0.05)	3.81 (-0.05)			13.78	14.55	260.48	-0.559
$MPMnI_3-1D-W$	0.000	20.0	1.07(-0.04)	1.07 (-0.04)	3.67	3.67	42.24	>1000	42.27	-0.227
NH_4GeBr_3-1D-W	0.000	0.0	3.24(-0.04)	3.25 (-0.04)			2.35	3.36	7.80	-0.570
$GPbCl_3-1D-W$	0.000	0.0	3.55(-0.61)	3.61 (-0.60)			3.55	3.76	64.81	-0.586
$MSTeBr_3-1D-W$	0.000	0.0	1.43(-0.00)	1.52 (-0.01)	2.31	2.42	8.15	10.33	38.51	-0.234
$MPMnCl_3-1D-W$	0.000	20.0	1.52(-0.00)	1.52 (-0.00)			44.46	>1000	44.46	-0.467
NH_4PdCl_3	0.000	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.556
NH_4CaBr_3-1D-R	0.000	0.0	4.10(-0.10)	4.10 (-0.10)			0.34	0.35	6.64	-1.056
$MPGeCl_3-3D-OR$	0.000	0.0	3.09(-0.03)	3.09 (-0.03)			0.52	1.09	0.99	-0.415
H_3STeBr_3-1D-W	0.000	0.0	1.05(-0.02)	1.05 (-0.02)	1.87	1.87	363.95	>1000	417.06	-0.231
$H_3SAuI_3-3D-OR$	0.000	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.100
NH_4AuI_3-1D-W	0.000	0.0	0.54(-0.15)	0.56 (-0.14)	1.26	1.30	10.15	42.32	13.36	-0.317
$NH_4TlBr_3-3D-OR$	0.000	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00	0.63	0.94	1.88	-0.545
$MPCaBr_3-1D-W$	0.000	0.0	4.07(-0.03)	4.07 (-0.03)			0.64	0.68	10.54	-0.679
$MPSnCl_3$	0.000	0.0	2.47(-0.17)	2.47 (-0.18)			0.42	1.23	0.64	-0.457
NH_4CaI_3-1D-W	0.000	0.0	3.52(-0.29)	3.53 (-0.28)			7.80	46.03	9.39	-0.852
NH_4AuCl_3-1D-W	0.000	0.0	1.09(-0.20)	1.09 (-0.19)	2.26	2.27	40.75	49.20	237.09	-0.514
NH_4SnBr_3-1D-R	0.000	0.0	2.23(-0.06)	2.40 (-0.07)			1.84	4.32	3.20	-0.635

Table ESI-2 Continuation of Table ESI-1

			PBE gap		HSE gap					
composition	E_{hull}	μ/μ_B	fund.	direct	fund.	direct	m^*	m_e^*	m_h^*	E_{f}
$GCaBr_3-1D-W$	0.000	0.0	4.55(-0.05)	4.56 (-0.04)			0.84	1.01	5.18	-0.759
NH_4SnCl_3-1D-W	0.000	0.0	3.56(-0.05)	3.58 (-0.05)			2.27	2.45	30.80	-0.750
NH_4SnI_3-1D-R	0.000	0.0	1.87(-0.15)	1.90 (-0.17)			1.76	9.12	2.19	-0.479
NH_4PbCl_3-1D-R	0.000	0.0	2.87(-0.44)	3.07 (-0.44)			3.52	5.64	9.39	-0.802
NH_4AgCl_3	0.000	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.541
$MPSrI_3-1D-W$	0.000	0.0	3.32(-0.20)	3.32 (-0.20)			0.55	0.55	40.79	-0.549
$GSnI_3-1D-W$	0.000	0.0	2.65(-0.14)	2.71 (-0.11)			1.99	4.88	3.36	-0.386
H_3SGeCl_3-2D	0.000	0.0	3.32(-0.01)	3.65 (-0.01)			2.73	3.04	27.21	-0.499
$MPBeBr_3-1D-W$	0.000	0.0	4.33(-0.07)	4.35 (-0.09)			1.10	1.11	160.36	-0.433
$NH_4FeBr_3-1D-W\bullet$	0.000	16.0	0.00(-0.01)	0.00 (-0.01)	2.51	2.57	>1000	>1000	>1000	-0.509
NH_4BeCl_3-1D-W	0.000	0.0	4.94(-0.00)	4.98 (-0.00)			0.56	0.56	353.87	-0.887
$MPGeCl_3$	0.000	0.0	2.96(-0.03)	2.96 (-0.02)			0.51	0.83	1.32	-0.415
$NH_4CdCl_3-1D-R\bullet$	0.000	0.0	3.51(-0.02)	3.62 (-0.02)			0.42	0.43	10.10	-0.776
$NH_4PbI_3-1D-R\bullet$	0.000	0.0	1.88(-0.63)	1.88 (-0.63)			2.50	7.51	3.76	-0.528
$GZnBr_3$	0.000	0.0	3.04(-0.05)	3.08 (-0.06)	4.34	4.38	0.54	0.55	25.10	-0.497
$MPSnCl_3-3D-OR$	0.001	0.0	2.27(-0.21)	2.27 (-0.21)			0.29	0.80	0.46	-0.457
$MPAuI_3-3D-OR$	0.001	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.155
$MPSnBr_3$	0.001	0.0	1.80(-0.23)	1.80 (-0.20)	2.78	2.83	0.39	1.03	0.63	-0.372
H_3SCaBr_3-1D-R	0.001	0.0	4.20(-0.09)	4.20 (-0.09)			1.96	1.97	277.12	-0.912
$H_3SInCl_3-3D-OR$	0.001	0.0	1.41(-0.00)	2.16 (-0.01)	2.21	2.98	0.36	0.74	0.69	-0.564
NH_4HgCl_3-1D-W	0.001	0.0	2.71(-0.03)	2.72 (-0.03)			0.90	0.90	221.19	-0.604
$MPInCl_3-3D-OR$	0.001	0.0	1.50(-0.01)	2.20 (-0.01)	2.25	3.04	0.64	0.87	2.41	-0.447
$MPGeBr_3-3D-OR$	0.001	0.0	2.31(-0.05)	2.31 (-0.05)			0.37	0.62	0.90	-0.327
NH_4SnBr_3-1D-W	0.001	0.0	3.05(-0.07)	3.08 (-0.07)			1.78	2.27	8.31	-0.634
$MPGeBr_3$	0.001	0.0	2.44(-0.05)	2.44 (-0.05)			0.63	0.77	3.48	-0.326
NH_4AuBr_3-1D-W	0.001	0.0	0.70(-0.19)	0.71 (-0.18)	1.70	1.70	13.63	13.77	>1000	-0.420
NH_4ZnBr_3-1D-W	0.001	0.0	3.52(-0.09)	3.52 (-0.09)			0.45	0.46	26.56	-0.672
H_3SSrI_3-1D-R	0.001	0.0	3.39(-0.21)	3.39 (-0.21)			2.77	2.82	159.68	-0.721
H_3SSnBr_3-2D	0.002	0.0	2.28(-0.10)	2.47 (-0.13)			1.35	3.02	2.43	-0.438
$NH_4PbI_3-1D-W\bullet$	0.002	0.0	2.35(-0.75)	2.45 (-0.73)			2.35	2.82	14.09	-0.527
NH_4AuBr_3-2D	0.002	0.0	0.58(-0.04)	0.64 (-0.05)	1.22	1.31	6.54	18.35	10.17	-0.420
$MPPbCl_3-1D-W$	0.002	0.0	3.31(-0.42)	3.36 (-0.46)			0.93	0.94	180.35	-0.486
NH_4AuI_3-2D	0.002	0.0	0.25(-0.05)	0.25 (-0.08)	1.00	1.10	1.35	5.24	1.81	-0.315
$H_3SGeCl_3-3D-OR$	0.002	0.0	2.68(-0.05)	2.68 (-0.05)			0.45	1.47	0.64	-0.498
NH_4TlCl_3-1D-W	0.002	0.0	1.48(-0.00)	1.60 (-0.00)	2.45	2.56	3.79	3.80	935.51	-0.668
$MSAuBr_3-3D-OR$	0.002	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.211
$MPCdCl_3-1D-W$	0.002	0.0	3.73(-0.01)	3.73 (-0.01)			0.65	0.65	419.77	-0.465
NH_4SnI_3-1D-W	0.002	0.0	2.44(-0.18)	2.55 (-0.13)			1.63	2.97	3.61	-0.477
NH_4ZnCl_3-1D-W	0.002	0.0	3.95(-0.00)	3.95 (-0.00)			0.56	0.56	>1000	-0.796
$MPMnBr_3-1D-W$	0.002	20.0	1.38(-0.01)	1.38 (-0.01)			15.92	26.05	40.92	-0.358
NH_4MnCl_3-1D-W	0.002	20.0	1.14(-0.00)	1.17 (-0.00)			78.36	>1000	78.37	-0.758
$MPZnBr_3-1D-W$	0.002	0.0	3.15(-0.05)	3.15 (-0.05)			0.65	0.65	>1000	-0.399
NH_4MgCl_3-1D-W	0.003	0.0	4.83(-0.01)	4.83 (-0.01)			0.44	0.44	628.49	-1.024
NH_4SnCl_3-1D-R	0.003	0.0	2.63(-0.04)	2.92 (-0.04)			2.87	5.00	6.73	-0.747
H_3SGeBr_3-1D-W	0.003	0.0	3.33(-0.04)	3.44 (-0.05)			5.93	6.93	41.26	-0.369

Table ESI-3 Continuation of Table ESI-2

			PBE gap		HSE gap					
composition	E_{hull}	μ/μ_B	fund.	direct	fund.	direct	m^*	m_e^*	m_h^*	E_{f}
H_3SSnCl_3-1D-R	0.003	0.0	3.05(-0.04)	3.49 (-0.04)			10.07	15.00	30.67	-0.565
$tBASnI_3-1D-W$	0.003	0.0	2.55(-0.19)	2.60 (-0.20)			2.61	23.16	2.94	-0.298
$GGeF_3-1D-W$	0.003	0.0	4.72(-0.00)	4.72 (-0.00)			1.79	1.88	39.45	-0.942
$MSHgBr_3-1D-W$	0.003	0.0	2.33(-0.09)	2.33 (-0.09)			0.88	0.88	761.29	-0.290
NH_4GeI_3-1D-W	0.003	0.0	2.59(-0.13)	2.76 (-0.16)			0.75	0.94	3.76	-0.418
$GGeI_3-1D-W$	0.003	0.0	2.80(-0.13)	2.91 (-0.13)			1.57	2.23	5.36	-0.346
$MPSnBr_3-1D-W$	0.003	0.0	2.78(-0.05)	2.88 (-0.05)			0.74	0.86	5.59	-0.370
$MPSnI_3-1D-W$	0.003	0.0	2.01(-0.10)	2.16 (-0.12)			0.51	0.55	6.55	-0.260
NH_4InCl_3-1D-W	0.003	0.0	2.16(-0.00)	2.35 (-0.00)			1.81	1.81	>1000	-0.747
$H_3SGeBr_3-3D-OR$	0.003	0.0	1.76(-0.06)	1.76 (-0.06)	2.36	2.36	0.23	0.58	0.37	-0.368
$H_3SSnBr_3-3D-OR$	0.004	0.0	1.26(-0.29)	1.26 (-0.29)	1.67	1.67	0.22	0.77	0.30	-0.436
NH_4AgBr_3	0.004	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.445
NH_4MnBr_3-1D-W	0.004	20.0	1.32(-0.01)	1.33 (-0.01)			14.03	>1000	14.09	-0.627
H_3SGeCl_3-1D-R	0.004	0.0	3.51(-0.01)	3.75 (-0.01)			3.95	4.33	45.11	-0.496
H_3SGeCl_3-1D-W	0.004	0.0	3.67(-0.01)	3.73 (-0.02)			7.36	7.80	131.74	-0.496
$MPGeBr_3-1D-W$	0.004	0.0	2.95(-0.03)	3.04 (-0.03)			0.71	0.83	4.86	-0.323
$tBAHgBr_3-1D-W$	0.004	0.0	2.39(-0.08)	2.39 (-0.08)			2.15	2.15	>1000	-0.320
H_3SZnCl_3-1D-W	0.004	0.0	3.84(-0.00)	3.84 (-0.00)			0.90	0.90	>1000	-0.618
NH_4GeCl_3-1D-W	0.004	0.0	3.78(-0.01)	3.89 (-0.01)			2.91	3.44	18.86	-0.689
H_3SPbBr_3-2D	0.004	0.0	2.20(-0.63)	2.33 (-0.65)			0.63	0.94	1.88	-0.495
$MSPbBr_3-1D-R$	0.004	0.0	2.52(-0.50)	2.58 (-0.51)			44.28	149.35	62.93	-0.418
$MPHgBr_3-1D-W$	0.005	0.0	2.30(-0.09)	2.30 (-0.09)			0.77	0.77	>1000	-0.285
$MPFeBr_3-1D-W$	0.005	16.0	0.00(-0.01)	0.00 (-0.01)	2.65	2.65	>1000	>1000	>1000	-0.271
$H_3SSnCl_3-3D-OR$	0.005	0.0	2.05(-0.23)	2.06 (-0.22)			0.37	1.25	0.53	-0.564
NH_4AuCl_3-2D	0.005	0.0	0.77(-0.09)	0.78 (-0.10)	1.53	1.56	2.29	37.53	2.44	-0.509
NH_4CaI_3-1D-R	0.005	0.0	3.33(-0.25)	3.33 (-0.25)			0.35	0.38	4.14	-0.847
$GBaI_3-1D-W$	0.005	0.0	3.54(-0.29)	3.54 (-0.29)			3.93	130.12	4.05	-0.643
H_3SSnCl_3-2D	0.005	0.0	2.72(-0.06)	3.04 (-0.06)			3.02	5.20	7.22	-0.563
H_3SCdI_3	0.005	0.0	1.81(-0.24)	1.81 (-0.24)			0.32	0.32	39.23	-0.296
$MSAuBr_3-1D-W$	0.005	0.0	0.24(-0.26)	0.26 (-0.25)	1.23	1.24	315.48	519.74	802.75	-0.208
$NH_4AuBr_3-3D-OR$	0.005	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.416
NH_4PbBr_3-1D-W	0.005	0.0	2.98(-0.53)	3.01 (-0.51)			1.97	2.82	6.58	-0.681
NH_4CaCl_3-2D	0.005	0.0	5.02(-0.02)	5.02 (-0.02)			0.47	0.49	13.15	-1.206
$MPZnCl_3-1D-W$	0.005	0.0	3.97(-0.00)	3.97 (-0.00)			0.81	0.81	812.91	-0.476
NH_4PbCl_3-2D	0.005	0.0	2.68(-0.54)	2.79 (-0.54)			0.63	0.94	1.88	-0.797
$MPCaBr_3-1D-R$	0.005	0.0	3.68(-0.06)	3.68 (-0.06)			193.70	194.58	>1000	-0.674
$tBABeCl_3-1D-W$	0.005	0.0	5.14(-0.00)	5.17 (-0.00)			0.65	0.65	>1000	-0.474
H_3SGeCl_3	0.005	0.0	1.96(-0.03)	1.96 (-0.03)	2.55	2.55	0.28	1.07	0.37	-0.494
$MPSnI_3-3D-OR$	0.005	0.0	0.73(-0.30)	0.73 (-0.30)	1.18	1.18	0.16	0.64	0.22	-0.257
$MSPbBr_3-2D$	0.005	0.0	2.27(-0.62)	2.47 (-0.56)			1.41	1.88	5.64	-0.417
$MPPbBr_3-3D-OR$	0.005	0.0	1.09(-1.07)	1.09 (-1.07)			0.20	0.52	0.32	-0.402
NH_4CoBr_3-1D-W	0.006	12.0	0.00(0.00)	0.00 (0.00)	3.38	3.39	77.80	654.70	88.30	-0.453
$MPPbBr_3-1D-W$	0.006	0.0	2.87(-0.35)	2.93 (-0.41)			0.69	0.74	9.68	-0.402
NH_4SnBr_3-2D	0.006	0.0	1.98(-0.12)	2.12 (-0.12)			0.54	1.25	0.94	-0.629
NH_4SnCl_3-2D	0.006	0.0	2.42(-0.09)	2.59 (-0.09)			0.68	1.39	1.34	-0.744

Table ESI-4 Continuation of Table ESI-3

			PBE gap		HSE gap					
composition	E_{hull}	μ/μ_B	fund.	direct	fund.	direct	m^*	m_e^*	m_h^*	E_{f}
$MPPbCl_3-3D-OR$	0.006	0.0	1.58(-1.04)	1.58 (-1.04)			0.24	0.71	0.37	-0.482
$NH_4CdBr_3-1D-R\bullet$	0.006	0.0	2.64(-0.09)	2.69 (-0.13)			0.31	0.33	7.88	-0.658
$MPPbCl_3$	0.006	0.0	2.10(-0.91)	2.10 (-0.91)			1.82	1.88	61.06	-0.481
$MPPbBr_3$	0.006	0.0	1.49(-0.93)	1.49 (-0.93)			1.46	1.88	6.58	-0.401
NH_4MgBr_3-1D-W	0.006	0.0	4.13(-0.06)	4.13 (-0.06)			0.34	0.36	6.12	-0.868
H_3SSnCl_3-1D-W	0.006	0.0	3.51(-0.04)	3.55 (-0.04)			3.61	3.63	962.91	-0.562
$GGeCl_3-1D-W$	0.006	0.0	4.18(-0.01)	4.22 (-0.01)			3.03	3.18	63.68	-0.523
$H_3SGeF_3-3D-OR$	0.006	0.0	4.35(-0.03)	4.37 (-0.02)			1.00	2.15	1.86	-1.220
H_3SCdI_3-1D-W	0.006	0.0	2.43(-0.20)	2.43 (-0.24)			0.62	0.63	84.35	-0.295
NH_4GeBr_3-1D-R	0.007	0.0	2.41(-0.03)	2.54 (-0.04)			3.30	14.39	4.29	-0.564
NH_4PbBr_3-2D	0.007	0.0	2.16(-0.60)	2.22 (-0.60)			0.47	0.94	0.94	-0.680
$NH_4CaCl_3-3D-OR$	0.007	0.0	4.78(-0.00)	4.90 (-0.00)			0.47	0.48	22.13	-1.205
$MPGeCl_3-1D-W$	0.007	0.0	3.62(-0.00)	3.73 (-0.00)			1.09	1.13	32.22	-0.408
$MPSnI_3$	0.007	0.0	0.89(-0.27)	0.89 (-0.27)	1.35	1.35	0.52	0.89	1.23	-0.256
H_3SSnBr_3-1D-W	0.007	0.0	3.07(-0.05)	3.12 (-0.06)			2.65	2.94	27.44	-0.432
$MSSrI_3-1D-R$	0.007	0.0	3.15(-0.21)	3.15 (-0.21)			108.80	148.61	406.09	-0.578
$MPPbBr_3-1D-R$	0.007	0.0	2.46(-0.43)	2.60 (-0.44)			50.53	116.47	89.23	-0.400
$MPZnCl_3-2D$	0.007	0.0	3.91(-0.01)	3.92 (-0.01)			1.58	1.58	>1000	-0.474
$GSnCl_3-3D-OR$	0.007	0.0	2.48(-0.13)	2.48 (-0.13)			0.44	1.61	0.60	-0.552
NH_4AgBr_3-2D	0.007	0.0	0.11(-0.03)	0.30 (-0.04)	0.73	0.92	0.06	0.12	0.12	-0.441
$NH_4HgCl_3-3D-OR$	0.007	0.0	1.97(-0.02)	2.38 (-0.02)	3.19	3.71	0.63	0.75	4.11	-0.597
$EASnI_3-1D-W$	0.007	0.0	2.48(-0.14)	2.53 (-0.17)			2.09	3.76	4.70	-0.344
NH_4SrCl_3-1D-R	0.007	0.0	5.00(-0.02)	5.00 (-0.02)			0.43	0.44	18.19	-1.228
H_3SCaBr_3-2D	0.007	0.0	4.24(-0.10)	4.24 (-0.13)			1.41	1.59	12.74	-0.905
$MSZnBr_3-1D-W$	0.008	0.0	3.28(-0.05)	3.28 (-0.05)			0.68	0.68	>1000	-0.407
$tBABeBr_3-1D-W$	0.008	0.0	4.42(-0.08)	4.43 (-0.09)			0.32	0.32	>1000	-0.399
NH_4MnCl_3	0.008	5.0	1.02(-0.00)	1.65 (0.00)	3.52	5.61	0.68	2.03	1.03	-0.753
H_3SGeBr_3-1D-R	0.008	0.0	3.00(-0.05)	3.30 (-0.04)			6.19	8.52	22.62	-0.364
H_3SZnBr_3-1D-W	0.008	0.0	3.50(-0.08)	3.52 (-0.10)			0.52	0.52	513.50	-0.479
$NH_4PbI_3-2D\bullet$	0.008	0.0	1.64(-0.77)	1.64 (-0.77)			0.70	2.82	0.94	-0.521
$MSPbBr_3-1D-W$	0.008	0.0	2.83(-0.40)	2.88 (-0.43)			0.87	0.94	11.27	-0.415
$MPCaI_3-1D-R$	0.008	0.0	3.07(-0.18)	3.07 (-0.18)			231.08	242.47	>1000	-0.526
NH_4CaBr_3-2D	0.008	0.0	4.04(-0.12)	4.04 (-0.12)			0.36	0.38	7.60	-1.048
$GGeBr_3-1D-W$	0.008	0.0	3.54(-0.03)	3.56 (-0.04)			0.15	0.91	0.18	-0.445
$tBASrI_3-1D-W$	0.008	0.0	3.75(-0.18)	3.75 (-0.18)			0.60	0.61	73.62	-0.466
NH_4CuCl_3	0.008	0.0	0.00(0.00)	0.00 (0.00)	0.00	0.00				-0.564
$H_3SCdI_3-3D-OR$	0.008	0.0	1.97(-0.25)	1.98 (-0.24)			0.55	0.56	27.21	-0.293
NH_4AgCl_3-2D	0.008	0.0	0.31(-0.00)	0.43 (-0.00)	1.31	1.44	1.61	3.20	3.22	-0.533
$NH_4SnF_3-3D-OR$	0.008	0.0	3.74(-0.02)	3.74 (-0.02)			0.88	1.36	2.51	-1.387
NH_4GeI_3-1D-R	0.008	0.0	1.96(-0.14)	2.01 (-0.17)			2.56	28.18	2.82	-0.413
$GSnBr_3-3D-OR$	0.008	0.0	1.95(-0.18)	1.95 (-0.18)			0.35	1.25	0.48	-0.476
$MSSeBr_3-3D-OR$	0.008	0.0	0.37(0.01)	0.38 (0.00)	1.54	1.55	26.86	68.57	44.15	-0.187
$MPBeCl_3$	0.008	0.0	4.90(-0.01)	5.01 (-0.00)			0.90	0.93	35.12	-0.552
NH_4SnI_3-2D	0.008	0.0	1.59(-0.20)	1.65 (-0.23)	2.31	2.36	0.53	2.59	0.67	-0.471
H_3SZnCl_3-1D-R	0.008	0.0	3.99(-0.02)	4.00 (-0.03)			0.54	0.54	977.79	-0.614

Table ESI-5 Continuation of Table ESI-4

			PBE gap		HSE gap					
composition	E_{hull}	μ/μ_B	fund.	direct	fund.	direct	m^*	m_e^*	m_h^*	E_{f}
$GZnBr_3-1D-W$	0.008	0.0	3.60(-0.05)	3.60 (-0.05)			0.62	0.63	62.30	-0.489
$MSPbBr_3$	0.009	0.0	1.07(-0.96)	1.07 (-0.96)			0.25	0.84	0.35	-0.414
$MPMnI_3$	0.009	5.0	1.58(-0.19)	1.73 (-0.17)			10.69	63.79	12.85	-0.218
$GZnCl_3-1D-W$	0.009	0.0	4.50(-0.00)	4.50 (-0.00)			0.69	0.70	58.38	-0.582
$MPPbCl_3-1D-R$	0.009	0.0	2.85(-0.36)	3.12 (-0.37)			52.36	69.51	212.28	-0.479
H_3SPbCl_3-1D-R	0.009	0.0	2.92(-0.45)	3.13 (-0.45)			14.60	20.66	49.78	-0.623
$NH_4HgBr_3-3D-OR$	0.009	0.0	2.06(-0.07)	2.07 (-0.06)			0.69	0.74	8.61	-0.516
$MPCdBr_3-1D-W$	0.009	0.0	2.98(-0.06)	2.98 (-0.06)			0.54	0.54	73.85	-0.384
$MPSnCl_3-1D-W$	0.009	0.0	3.30(-0.02)	3.38 (-0.02)			0.87	0.88	74.22	-0.448
NH_4InBr_3-1D-W	0.009	-0.0	1.54(-0.01)	1.81 (-0.02)	2.43	2.69	1.07	1.11	33.31	-0.629
NH_4GeF_3	0.009	0.0	4.01(-0.02)	4.01 (-0.04)	5.13	5.14	0.61	1.33	1.11	-1.324
$MPMgCl_3-1D-W$	0.009	0.0	4.51(-0.00)	4.51 (-0.00)			0.65	0.70	9.27	-0.652
NH_4GeCl_3-2D	0.009	0.0	3.13(-0.04)	3.37 (-0.02)			1.18	2.26	2.49	-0.684
$MSCaBr_3-2D$	0.010	0.0	4.15(-0.13)	4.17 (-0.12)			1.04	1.12	14.48	-0.715
$MSTeBr_3-1D-R$	0.010	0.0	0.42(0.12)	0.44 (0.13)	1.53	1.55	54.27	122.11	97.69	-0.225
$H_3SZnCl_3-3D-OR$	0.010	0.0	3.94(-0.01)	3.95 (-0.01)			0.57	0.57	86.43	-0.613
$MPGeBr_3-2D$	0.010	0.0	3.16(-0.06)	3.28 (-0.05)			1.94	2.15	20.11	-0.318
$MPSrBr_3-3D-OR$	0.010	0.0	4.36(-0.08)	4.40 (-0.07)			0.60	0.64	8.28	-0.696
$GSnF_3-1D-W$	0.010	0.0	3.95(-0.01)	3.95 (-0.01)			1.41	1.88	5.64	-0.964
$NH_4CdBr_3-1D-W\bullet$	0.010	0.0	2.93(-0.10)	2.95 (-0.07)			0.42	0.43	16.03	-0.653
NH_4BeCl_3	0.010	0.0	5.01(-0.01)	5.14 (-0.00)	6.38	6.51	0.46	0.51	4.93	-0.877
$MPGeCl_3-2D$	0.010	0.0	3.44(-0.01)	3.71 (-0.01)			1.46	1.52	39.72	-0.405
$GZnI_3$	0.010	0.0	2.85(-0.16)	3.00 (-0.22)	3.94	4.07	0.60	0.65	7.61	-0.387