Supplementary Materials for: Exploring Flat-Band Properties in Two-Dimensional M_3QX_7 Compounds

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TABLE S1: Distance to the convex-hull ($E_{\rm hull}$ in eV), formation energy ($E_{\rm form}$ in eV), indirect band gap ($E_{\rm Gap}$ in eV), magnetization per metal atom (in $\mu_{\rm B}$), minimal dispersion ($D_{\rm min}$ in meV) of the band between –3.0 to +3.0 eV around Fermi level, and the mean eigenvalue of this flattest band relative to Fermi level ($\overline{E}$ in eV). Note the $D_{\rm min}$ values listed are calculated on a coarse k-grid and therefore are underestimated. All results obtained with the PBE functional. For completeness we also include the case where X and Q are the same chemical element, leading to the composition M_3X_8.

Formula	$E_{\rm hull}$	$E_{\rm form}$	$E_{\rm Gap}$	M	$D_{\rm min}$	$\overline{E}$
Fe_3I_8	-0.010	-0.07	0.02	4.5	36	0.533
V_3Cl_8	-0.008	-1.65	0.00	2.3	30	-0.140
V_3ICl_7	-0.007	-1.50	0.00	2.3	29	-0.119
Nb_3IBr_7	-0.004	-0.85	0.33	0.4	59	-0.875
Ti_3ICl_7	-0.001	-1.86	0.51	0.7	19	1.025
Ti_3BrCl_7	-0.001	-1.91	0.47	0.7	25	1.042
Nb_3BrCl_7	0.001	-1.60	0.24	0.3	29	-1.247
Nb_3Br_8	0.001	-0.90	0.34	0.4	58	-0.895
Ti_3Cl_8	0.001	-2.01	0.43	0.7	37	1.364
V_3Br_8	0.002	-0.86	0.00	2.3	26	2.235
Ti_3TeCl_7	0.003	-1.86	0.64	1.0	15	-2.390
V_3I_8	0.003	-0.46	0.00	2.3	33	2.218
Nb_3Cl_8	0.003	-1.70	0.25	0.3	20	-1.277
Nb_3TeCl_7	0.003	-1.58	0.75	0.0	20	-0.267
Mn_3Cl_8	0.003	-1.40	0.00	4.3	35	1.576
Nb_3ICl_7	0.003	-1.55	0.21	0.3	51	-1.226
Nb_3TeBr_7	0.004	-0.88	0.70	0.0	54	2.548
Nb_3SeCl_7	0.004	-1.64	0.80	0.0	20	-0.254
Zr_3ICl_7	0.004	-1.99	0.55	0.6	48	-0.218
Nb_3SCl_7	0.005	-1.73	0.85	0.0	23	-0.247
Nb_3I_8	0.006	-0.50	0.29	0.3	39	-0.896
Nb_3TeI_7	0.007	-0.52	0.61	0.0	30	-0.151
Nb_3SBr_7	0.007	-1.03	0.79	0.0	74	2.881
Fe_3Cl_8	0.009	-1.14	0.00	4.7	25	0.373
V_3TeCl_7	0.010	-1.47	0.07	2.0	11	1.988
Ti_3Br_8	0.011	-1.19	0.40	0.6	20	0.999
Zr_3BrCl_7	0.012	-2.04	0.54	0.7	30	-0.192
Zr_3IBr_7	0.012	-1.29	0.61	0.7	48	-0.157
Sc_3I_8	0.013	-1.20	0.00	0.4	32	0.889
Ta_3TeI_7	0.013	-0.43	0.67	0.0	42	-0.154
Ni_3Cl_8	0.015	-0.91	0.00	1.3	103	-2.391
Ta_3SeI_7	0.015	-0.49	0.70	0.0	29	-0.152
Zr_3TeCl_7	0.017	-1.98	0.37	1.0	11	-2.563
Zr_3Cl_8	0.017	-2.13	0.55	0.7	21	-0.162
Sc_3IBr_7	0.018	-1.60	0.00	0.4	26	0.968
Mn_3Br_8	0.020	-0.67	0.00	4.3	17	1.672
Sc_3Br_8	0.020	-1.65	0.00	0.4	22	1.029
Zr_3Br_8	0.021	-1.33	0.62	0.7	34	-0.137
Mn_3I_8	0.021	-0.33	0.00	4.3	27	1.472
In_3SeCl_7	0.022	-1.37	2.84	0.0	81	-0.764
Sc_3BrCl_7	0.022	-2.37	0.00	0.4	30	1.008
Sc_3ICl_7	0.023	-2.31	0.00	0.4	39	0.994
Ti_3I_8	0.023	-0.74	0.00	1.3	23	1.460
Sc_3TeBr_7	0.024	-1.62	2.05	0.0	51	2.732
Sc_3Cl_8	0.024	-2.47	0.00	0.4	27	1.009
Zr_3I_8	0.025	-0.90	0.56	0.7	40	-0.278
Zr_3SeCl_7	0.025	-2.04	0.43	1.0	16	-2.933
Sc_3SeCl_7	0.027	-2.41	2.81	0.0	29	-0.114
Sc_3TeCl_7	0.028	-2.33	2.20	0.0	22	-0.380
Ta_3TeCl_7	0.028	-1.52	0.80	0.0	30	-0.287
Zr_3TeBr_7	0.030	-1.28	0.40	1.0	35	-2.424
Pm_3I_8	0.032	-1.35	0.00	0.3	76	-2.465
Y_3TeBr_7	0.032	-1.79	2.78	0.0	33	-2.636
Ni_3Br_8	0.032	-0.25	0.00	1.3	70	-0.570
Er_3TeBr_7	0.033	-1.77	2.90	0.0	51	-2.402
Fe_3Br_8	0.033	-0.41	0.00	4.7	11	0.309
Ho_3TeBr_7	0.033	-1.78	2.87	0.0	49	-2.444
Dy_3TeBr_7	0.034	-1.78	2.86	0.0	28	-2.417
Tb_3TeBr_7	0.034	-1.78	2.84	0.0	22	-2.405
Y_3SeCl_7	0.035	-2.57	3.42	0.0	12	-2.388
Sm_3TeBr_7	0.035	-1.78	2.77	0.1	18	-0.109
Pm_3TeBr_7	0.035	-1.78	2.74	0.1	18	-2.186
Cu_3F_8	0.036	-1.68	0.06	1.7	25	0.855
Tb_3SeCl_7	0.036	-2.57	3.47	0.0	26	-0.120
Dy_3SeCl_7	0.036	-2.57	3.51	0.0	27	-0.119
Hf_3IBr_7	0.036	-1.19	0.56	0.6	69	-0.295
Pd_3Cl_8	0.036	-0.79	0.00	0.7	112	-1.211
Ru_3I_8	0.036	-0.03	0.00	0.7	48	-0.299
Y_3I_8	0.037	-1.34	0.00	0.3	85	-2.516
Ho_3SeCl_7	0.037	-2.57	3.55	0.0	17	-2.438
In_3TeCl_7	0.037	-1.33	2.44	0.0	34	-0.935
Er_3SeCl_7	0.037	-2.57	3.60	0.0	8	-2.445
Tm_3SeCl_7	0.037	-2.57	3.65	0.0	22	-2.465
Y_3TeCl_7	0.038	-2.50	2.94	0.1	35	-0.193
Y_3SCl_7	0.038	-2.66	3.72	0.0	5	-2.107
Er_3TeCl_7	0.039	-2.49	3.06	0.0	31	-0.216
Tm_3TeCl_7	0.039	-2.49	3.08	0.0	23	-2.943
Ho_3TeCl_7	0.039	-2.49	3.04	0.0	37	-2.584
Dy_3TeCl_7	0.040	-2.49	3.02	0.1	36	-2.547
Tb_3TeCl_7	0.040	-2.49	3.00	0.1	39	-2.508
Tb_3SCl_7	0.040	-2.66	3.78	0.0	19	-2.122

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Dy_3SCl_7	0.040	-2.66	3.81	0.0	20	-2.130
Tb_3I_8	0.040	-1.33	0.00	0.1	76	2.034
Ho_3SCl_7	0.040	-2.66	3.85	0.0	7	-2.149
Sm_3SeCl_7	0.040	-2.55	3.36	0.0	13	-2.802
Sm_3I_8	0.041	-1.34	0.00	0.2	78	-2.481
Ce_3IBr_7	0.041	-1.69	0.00	1.3	2	1.186
Nd_3I_8	0.042	-1.35	0.00	0.3	74	-2.455
Nd_3TeBr_7	0.043	-1.78	2.71	0.1	8	-2.169
Ce_3Br_8	0.043	-1.75	0.00	1.3	1	1.193
Sm_3TeCl_7	0.043	-2.48	2.94	0.1	16	-0.114
Np_3I_8	0.043	-0.81	0.00	4.3	12	0.095
Hf_3ICl_7	0.044	-1.92	0.50	0.7	67	-0.362
Dy_3I_8	0.044	-1.32	0.00	0.0	89	-2.583
Ce_3ICl_7	0.044	-2.39	0.00	1.3	4	1.237
Rb_8O_3	0.045	-0.93	0.03	0.0	42	-1.449
Np_3TeCl_7	0.045	-1.89	0.00	4.0	6	-1.884
Mo_3TeCl_7	0.046	-1.17	0.00	0.3	69	-1.508
Ce_3Cl_8	0.046	-2.54	0.00	1.3	8	-0.071
Ce_3BrCl_7	0.047	-2.44	0.00	1.3	3	1.246
Tc_3I_8	0.047	0.05	0.03	1.7	80	0.048
Ni_3I_8	0.047	-0.02	0.00	1.3	49	-1.456
Ho_3I_8	0.048	-1.31	0.00	0.0	80	2.015
Pd_3Br_8	0.049	-0.21	0.00	0.7	81	-2.353
Pr_3I_8	0.049	-1.36	0.00	0.3	71	-2.452
Hf_3TeCl_7	0.049	-1.92	0.00	0.3	19	-2.917
Hf_3Br_8	0.050	-1.24	0.56	0.6	51	-0.250
Cr_3Cl_8	0.050	-1.47	0.00	3.3	55	1.617
Hf_3I_8	0.050	-0.79	0.59	0.6	34	2.610
Pr_3TeBr_7	0.050	-1.78	2.69	0.1	6	-2.151
Hf_3TeBr_7	0.050	-1.19	0.00	0.4	72	-0.156
Pm_3SeCl_7	0.051	-2.55	3.33	0.0	21	-0.124
Cr_3Br_8	0.051	-0.70	0.00	3.3	14	1.869
Pm_3Br_8	0.051	-1.77	0.00	0.3	76	2.142
Pm_3IBr_7	0.052	-1.72	0.00	0.3	50	2.301
Y_3IBr_7	0.052	-1.72	0.00	0.3	61	2.195
Er_3I_8	0.052	-1.30	0.00	0.0	81	2.299
Pm_3TeCl_7	0.054	-2.48	2.91	0.1	14	-0.262
Sm_3IBr_7	0.055	-1.72	0.00	0.3	29	1.949
Hf_3BrCl_7	0.056	-1.97	0.47	0.7	41	-0.335
Y_3Br_8	0.057	-1.78	0.00	0.3	47	2.105
Sm_3Br_8	0.057	-1.77	0.00	0.3	74	2.162
Np_3IBr_7	0.057	-1.20	0.00	4.3	13	2.975
Cr_3I_8	0.057	-0.34	0.00	3.3	22	1.671
Tb_3IBr_7	0.058	-1.72	0.00	0.3	53	2.408
Tm_3I_8	0.058	-1.29	0.00	0.0	76	2.307
Pd_3F_8	0.058	-1.48	0.06	0.8	91	-2.755
Hg_3F_8	0.059	-1.45	0.00	0.6	18	-0.647
Np_3Br_8	0.060	-1.25	0.00	4.3	13	2.232
Nd_3IBr_7	0.060	-1.72	0.00	0.3	55	2.281
Np_3ICl_7	0.060	-1.90	0.00	4.3	10	2.230
Nd_3Br_8	0.061	-1.77	0.00	0.3	109	2.100
Dy_3IBr_7	0.061	-1.71	0.00	0.2	87	2.342
La_3I_8	0.063	-1.44	0.00	0.4	2	0.530
Tb_3Br_8	0.063	-1.77	0.00	0.3	84	2.058
Np_3BrCl_7	0.064	-1.95	0.00	4.3	12	1.928
In_3I_8	0.064	-0.42	0.00	0.0	112	-1.411
Np_3Cl_8	0.065	-2.05	0.00	4.3	14	-0.308
Ho_3IBr_7	0.066	-1.70	0.00	0.2	73	2.392
Zr_3SCl_7	0.067	-2.11	0.00	0.0	159	1.122
Y_3ICl_7	0.067	-2.42	0.00	0.3	47	2.397
Hf_3Cl_8	0.067	-2.06	0.45	0.6	20	-0.290
Dy_3Br_8	0.067	-1.76	0.00	0.3	73	2.084
Nd_3TeCl_7	0.069	-2.47	2.88	0.1	10	-0.269
Er_3IBr_7	0.070	-1.70	0.00	0.2	68	2.399
Y_3BrCl_7	0.071	-2.48	0.00	0.3	72	2.960
Ta_3I_8	0.071	-0.38	0.24	0.3	23	-0.787
Ho_3Br_8	0.071	-1.76	0.00	0.3	109	1.695
Sm_3ICl_7	0.072	-2.41	0.00	0.3	36	2.370
Pr_3IBr_7	0.072	-1.72	0.00	0.3	62	2.261
Tb_3ICl_7	0.072	-2.42	0.00	0.3	41	2.401
Ru_3Br_8	0.073	-0.21	0.00	0.7	66	0.377
La_3IBr_7	0.073	-1.82	0.40	0.4	2	0.512
Sm_3BrCl_7	0.073	-2.46	0.00	0.3	143	2.153
Ce_3TeCl_7	0.073	-2.40	0.08	1.0	2	-0.060
Y_3Cl_8	0.074	-2.58	0.00	0.3	102	2.945
Co_3Br_8	0.075	-0.24	0.00	0.3	79	-0.209
Dy_3ICl_7	0.075	-2.42	0.00	0.3	43	2.412
Tm_3IBr_7	0.075	-1.69	0.00	0.2	60	1.717
Pm_3ICl_7	0.075	-2.41	0.00	0.3	52	2.362
Er_3Br_8	0.076	-1.75	0.00	0.3	45	1.703
Co_3Cl_8	0.076	-0.94	0.00	0.3	70	-0.394
Sm_3Cl_8	0.076	-2.56	0.00	0.3	161	2.192
Pr_3Br_8	0.076	-1.77	0.00	0.3	121	2.065
Ru_3Cl_8	0.077	-0.88	0.00	0.7	80	-0.635
Tb_3BrCl_7	0.077	-2.47	0.00	0.3	118	2.065
Pm_3BrCl_7	0.079	-2.47	0.00	0.3	119	2.122
Ho_3ICl_7	0.079	-2.41	0.00	0.3	47	2.405
Dy_3BrCl_7	0.080	-2.47	0.00	0.3	149	2.592
Tb_3Cl_8	0.080	-2.57	0.00	0.3	173	2.103
Co_3F_8	0.081	-2.16	0.00	3.7	25	2.225
Tm_3Br_8	0.081	-1.74	0.00	0.2	35	1.718
La_3Br_8	0.083	-1.87	0.35	0.4	1	0.547
Pr_3TeCl_7	0.083	-2.47	2.86	0.1	6	-0.275
Dy_3Cl_8	0.083	-2.57	0.00	0.3	146	2.128
Er_3ICl_7	0.084	-2.41	0.00	0.3	52	2.405
Pm_3Cl_8	0.084	-2.56	0.00	0.3	171	2.170
Ho_3BrCl_7	0.084	-2.47	0.00	0.3	136	2.600
Ni_3F_8	0.084	-1.74	0.00	2.7	66	-1.492
As_3Br_8	0.084	-0.35	0.78	0.3	31	2.373
Sn_3I_8	0.086	-0.35	0.00	0.0	76	2.884
Ta_3Br_8	0.087	-0.80	0.28	0.3	75	-0.925
Ho_3Cl_8	0.087	-2.56	0.00	0.3	174	1.792
Pt_3Br_8	0.088	-0.13	0.00	0.7	56	-1.165
Tl_3Br_8	0.088	-0.43	0.00	0.0	62	-1.424
Er_3BrCl_7	0.088	-2.46	0.00	0.3	177	2.195
Co_3I_8	0.089	-0.00	0.00	0.3	86	-0.924
Tm_3ICl_7	0.089	-2.40	0.00	0.3	58	2.526
Tl_8S_3	0.090	-0.37	0.09	0.0	127	-1.578
La_3TeCl_7	0.091	-2.58	2.76	0.1	3	2.682
Er_3Cl_8	0.092	-2.56	0.00	0.3	160	1.818
Tl_3Cl_8	0.092	-1.04	0.00	0.0	11	-2.024
Nd_3ICl_7	0.093	-2.41	0.00	0.3	50	2.330
Bi_3Br_8	0.093	-0.63	0.00	0.0	39	1.375
Nd_3BrCl_7	0.094	-2.46	0.00	0.3	131	2.078
Tm_3BrCl_7	0.094	-2.46	0.00	0.3	127	2.622
Pd_3I_8	0.094	-0.09	0.00	0.5	46	-1.504
Bi_3IBr_7	0.095	-0.59	0.00	0.0	66	1.277
Pb_3Cl_8	0.096	-1.25	0.00	0.4	35	-0.787
Zn_3F_8	0.096	-2.10	0.00	0.7	22	-0.605
Nd_3Cl_8	0.097	-2.56	0.00	0.3	181	2.595
In_3Br_8	0.097	-0.71	0.00	0.0	65	-2.377
Tm_3Cl_8	0.097	-2.56	0.00	0.3	143	1.853
La_3ICl_7	0.097	-2.52	0.39	0.4	10	0.453
Bi_3BrCl_7	0.099	-1.21	0.00	0.0	78	1.538
Hf_3BiCl_7	0.100	-1.78	0.18	0.0	47	-1.978
Zr_3SbCl_7	0.100	-1.85	0.00	0.7	56	1.002
Bi_3Cl_8	0.100	-1.29	0.00	0.0	31	-2.988
Rb_8Cd_3	0.101	0.07	0.00	0.0	57	1.564

Pt_3Cl_8	0.101	-0.72	0.00	0.7	83	-1.309
Bi_3ICl_7	0.102	-1.17	0.00	0.0	54	1.423
Tl_8Se_3	0.103	-0.20	0.21	0.0	125	-1.346
Rb_8Hg_3	0.103	-0.04	0.00	0.0	63	1.582
La_3BrCl_7	0.103	-2.56	0.34	0.4	5	0.650
Pt_3I_8	0.104	-0.04	0.00	0.7	56	-1.053
Cu_3Cl_8	0.106	-0.72	0.00	1.2	21	-1.263
Pr_3ICl_7	0.106	-2.40	0.00	0.3	40	2.936
Pr_3BrCl_7	0.106	-2.45	0.00	0.3	123	2.871
Tl_3F_8	0.109	-2.04	0.00	0.0	125	1.449
Ta_3Cl_8	0.109	-1.62	0.16	0.3	35	-1.165
Pr_3Cl_8	0.109	-2.55	0.00	0.3	134	2.849
K_8Ag_3	0.110	0.11	0.00	0.0	117	0.923
V_3F_8	0.111	-3.04	0.00	2.3	38	-0.076
Tl_3ClF_7	0.112	-1.91	0.00	0.0	30	-2.863
Sb_3Br_8	0.113	-0.48	0.00	0.0	60	1.366
In_3Cl_8	0.115	-1.40	0.00	0.0	136	0.269
Sn_3Br_8	0.115	-0.60	0.00	0.0	53	-1.084
In_3BrCl_7	0.116	-1.31	0.00	0.0	161	0.253
K_8Hg_3	0.116	-0.03	0.00	0.0	113	1.670
Rb_8Na_3	0.117	0.12	0.00	0.0	102	0.468
Ag_3Cl_8	0.117	-0.57	0.00	0.9	23	-1.031
Ge_3I_8	0.119	-0.17	0.00	0.0	47	-2.369
Mo_3Cl_8	0.120	-1.21	0.20	0.7	77	-2.043
In_3ICl_7	0.121	-1.27	0.00	0.0	201	0.203
K_8Cd_3	0.121	0.08	0.00	0.0	97	2.428
As_3I_8	0.122	-0.05	0.00	0.0	84	1.005
Cr_3F_8	0.123	-2.86	0.00	3.3	24	0.425
Tl_8Au_3	0.124	0.09	0.00	0.0	145	-2.897
Cu_3Br_8	0.125	-0.11	0.00	0.0	124	-1.979
Au_3I_8	0.129	0.09	0.00	0.0	51	-1.257
Cu_3I_8	0.131	0.06	0.00	0.0	37	-1.905
Tc_3Br_8	0.133	-0.21	0.00	1.7	21	0.335
Hf_3SbCl_7	0.134	-1.81	0.00	0.7	71	1.283
Pb_3Br_8	0.134	-0.61	0.00	0.0	48	-0.444
Tl_8Te_3	0.136	-0.11	0.48	0.0	200	-1.028
Tl_8Sb_3	0.137	0.12	0.00	0.0	320	2.806
Mg_3I_8	0.138	-0.72	0.00	0.3	74	-0.758
Au_3Br_8	0.138	0.02	0.00	0.0	75	-1.610
Sn_3Cl_8	0.149	-1.25	0.00	0.0	33	-2.257
Al_3I_8	0.149	-0.48	0.00	0.0	104	-2.687
Sb_3ICl_7	0.149	-1.02	0.00	0.0	74	1.436
Cd_3Cl_8	0.151	-1.11	0.00	0.7	39	-0.977
Pb_3I_8	0.152	-0.38	0.00	0.0	57	-0.224
Hg_3Cl_8	0.152	-0.73	0.00	0.7	21	-1.218
Tl_3I_8	0.154	-0.21	0.00	0.0	68	-2.135
Ag_3Br_8	0.154	-0.03	0.00	0.0	47	-2.072
Mo_3Br_8	0.154	-0.44	0.03	0.7	48	0.735
Os_3Br_8	0.154	0.08	0.23	0.0	58	0.182
Hg_8F_3	0.156	-0.63	0.00	0.0	217	-2.867
Sb_3Cl_8	0.157	-1.13	0.00	0.0	66	-2.446
Zr_3HgCl_7	0.160	-1.75	0.12	1.0	25	-0.936
In_3F_8	0.160	-2.62	0.00	0.0	289	1.987
Tl_8As_3	0.161	0.16	0.00	0.0	141	-1.516
Ga_3I_8	0.161	-0.31	0.00	0.0	14	-2.924
Ga_3Hg_8	0.162	0.16	0.00	0.0	690	-2.059
Au_3Cl_8	0.165	-0.52	0.00	0.5	22	-1.324
Hg_8Au_3	0.165	0.16	0.00	0.0	350	-1.442
Fe_3F_8	0.166	-2.60	0.00	4.7	19	1.770
Mg_3Br_8	0.167	-1.05	0.00	0.7	53	-0.705
Zn_3Hg_8	0.168	0.17	0.00	0.0	656	-0.694
Cd_3I_8	0.169	-0.32	0.00	0.0	59	-1.520
Rb_8Li_3	0.169	0.17	0.00	0.0	49	0.916
Ge_3Br_8	0.171	-0.41	0.00	0.0	96	-0.763
K_8Li_3	0.173	0.17	0.00	0.0	82	0.526
Ca_3I_8	0.173	-1.16	0.00	0.7	45	-0.656
Ga_3Br_8	0.176	-0.62	0.00	0.0	115	-2.012
Os_3Cl_8	0.177	-0.61	0.00	0.0	149	-0.364
Zn_3Cl_8	0.179	-1.12	0.00	0.7	66	-1.329
Si_3Te_8	0.181	0.15	0.00	0.0	212	-1.513
Al_3H_8	0.182	0.06	0.00	0.0	1119	1.019
Rb_8H_3	0.183	0.06	0.00	0.1	14	-2.885
Cd_3Br_8	0.184	-0.52	0.00	0.7	83	-1.834
Ti_3F_8	0.184	-3.40	0.00	1.3	56	0.259
Al_3Br_8	0.185	-0.87	0.00	0.0	232	2.619
Hf_3HgCl_7	0.186	-1.68	0.00	0.0	29	-1.055
Tc_3Cl_8	0.187	-0.94	0.00	1.7	35	0.310
Hg_3Br_8	0.189	-0.18	0.00	0.6	47	-1.281
Nb_3HgCl_7	0.190	-1.32	0.41	0.0	30	-0.935
Te_8As_3	0.190	0.18	0.00	0.0	99	-1.652
Ga_3Cl_8	0.195	-1.32	0.00	0.0	626	0.181
K_8Cl_3	0.196	-1.03	0.00	0.0	283	1.628
Ag_3I_8	0.198	0.06	0.00	0.0	66	-1.876
As_3Se_8	0.198	0.11	0.00	0.0	69	-0.500
Ca_3Br_8	0.199	-1.47	0.06	0.7	25	-0.579
Rb_8F_3	0.199	-1.38	0.00	0.0	84	2.919
K_8H_3	0.201	0.05	0.00	0.1	154	2.744
Hg_3I_8	0.202	-0.04	0.00	0.0	76	-1.901
W_3Cl_8	0.202	-1.00	0.24	0.7	55	-2.530
Ga_3F_8	0.203	-2.66	0.00	0.0	158	2.027
Ru_3F_8	0.205	-1.64	0.00	0.7	22	-0.340
Ge_3Cl_8	0.208	-1.08	0.00	0.4	57	-1.904
Pb_3F_8	0.214	-2.33	0.00	0.0	14	-2.552
Se_3I_8	0.215	0.20	0.00	0.7	50	1.307
Ga_3Bi_8	0.217	0.22	0.00	0.0	675	-1.404
Ca_3Cl_8	0.217	-2.15	0.05	0.7	19	-0.838
Sb_3Te_8	0.219	0.13	0.00	0.0	123	-0.448
Ce_3F_8	0.219	-3.97	0.01	1.3	8	0.851
Mo_3I_8	0.219	-0.09	0.03	0.7	25	-2.195
K_8F_3	0.219	-1.39	0.00	0.0	267	1.436
Na_8H_3	0.224	0.08	0.00	0.0	443	0.756
Zn_3Br_8	0.225	-0.50	0.00	0.5	113	-2.127
Cu_3Te_8	0.226	0.19	0.00	0.0	87	-2.654
Al_3Cl_8	0.227	-1.67	0.00	0.0	198	2.509
Zr_3F_8	0.229	-3.43	0.80	0.6	71	-0.229
Zn_3I_8	0.231	-0.26	0.00	0.0	139	-1.844
As_3Cl_8	0.231	-0.90	0.00	0.0	85	1.562
Al_3Te_8	0.233	-0.08	0.00	0.0	290	-2.748
Tl_8F_3	0.233	-0.85	0.00	0.0	911	1.542
In_8Ge_3	0.237	0.24	0.00	0.0	570	1.038
W_3Br_8	0.238	-0.22	0.06	0.7	57	0.322
Li_3I_8	0.240	-0.42	0.00	0.0	274	-2.067
Bi_3F_8	0.242	-2.47	0.00	0.0	254	0.831
P_3Se_8	0.248	0.20	0.00	0.0	357	-0.722
Tc_3F_8	0.250	-1.88	0.47	1.7	14	-0.267
Sn_3Bi_8	0.250	0.25	0.00	0.0	563	-1.170
Sn_3Te_8	0.252	0.09	0.00	0.0	155	-1.182
Ga_3Au_8	0.253	0.12	0.00	0.0	556	-1.720
Te_8Au_3	0.253	0.18	0.00	0.0	221	-1.871
Se_3Cl_8	0.264	-0.48	0.00	0.7	16	-1.884
Na_8Br_3	0.267	-0.59	0.00	0.0	127	-0.298
Li_8H_3	0.270	0.01	0.00	0.0	326	-1.309
Na_8Cl_3	0.271	-0.88	0.00	0.0	324	-0.331
Te_3O_8	0.273	-1.12	0.00	0.0	114	-2.933
Cd_3Au_8	0.277	0.13	0.00	0.0	622	-0.258
Tl_8Cl_3	0.278	-0.44	0.00	0.0	467	2.560
Sn_3Se_8	0.278	-0.01	0.14	0.0	83	-1.184
Sb_3Se_8	0.286	0.11	0.00	0.0	167	-0.445

As_3S_8	0.296	-0.14	0.00	0.0	174	-0.535
Ga_3Te_8	0.297	0.07	0.00	0.0	366	-2.578
Na_3I_8	0.298	-0.39	0.00	0.0	239	-1.974
In_3Te_8	0.303	0.08	0.00	0.0	202	1.292
Ge_3Bi_8	0.306	0.31	0.00	0.0	532	-2.099
Si_3I_8	0.308	-0.03	0.00	0.0	125	-1.565
Ba_8H_3	0.310	0.07	0.00	0.0	47	0.366
Sb_3F_8	0.311	-2.32	0.00	0.0	29	-2.652
Re_3Br_8	0.317	0.08	0.22	1.7	55	-2.904
Bi_8Sb_3	0.319	0.31	0.00	0.0	314	-1.641
Ni_3Hg_8	0.319	0.32	0.00	0.0	53	-0.717
Be_3Cl_8	0.323	-1.21	0.00	0.6	340	-1.431
Be_3I_8	0.323	-0.14	0.00	0.0	288	-0.560
Hg_3Te_8	0.334	0.24	0.00	0.0	271	-0.960
P_3S_8	0.344	-0.30	0.00	0.0	190	-0.663
Zn_3Te_8	0.353	0.10	0.06	0.0	238	-0.477
Be_3Br_8	0.355	-0.48	0.00	0.0	291	-1.274
Al_3F_8	0.392	-3.38	0.00	0.0	381	2.308
I_3O_8	0.393	-0.32	0.00	0.0	84	-2.188
Hf_3F_8	0.402	-3.37	0.76	0.7	33	-0.759
H_3Pd_8	0.405	0.31	0.00	0.0	217	-2.875
As_3F_8	0.419	-2.00	0.00	0.0	91	-2.853
Re_3Cl_8	0.440	-0.64	0.34	1.7	28	-0.222
Si_3Br_8	0.444	-0.29	0.00	0.0	103	-2.833
P_3Cl_8	0.445	-0.66	0.00	0.0	86	-2.863
Ag_8Te_3	0.480	0.44	0.00	0.0	86	-1.391
Te_3Au_8	0.526	0.47	0.00	0.0	49	-2.420
B_3I_8	0.740	0.69	0.00	0.0	311	2.261

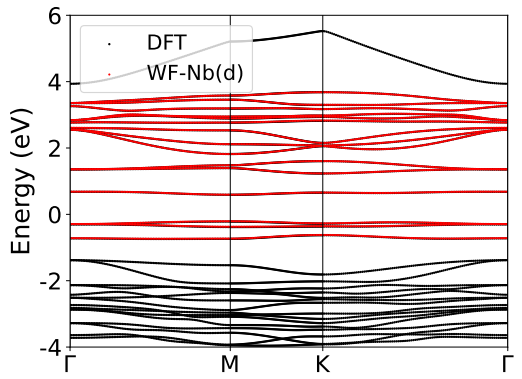

FIG. S1. Electronic band structure of Nb_3SBr_7 from DFT (black) and interpolated by the tight-binding model (red).

TABLE S2. Calculated elastic constants in N/m.

Formula	C_{11}	C_{12}	C_{22}	C_{66}
Nb_3SeCl_7	62.9	17.2	59.6	19.1
Nb_3TeCl_7	53.1	16.1	53.3	18.5
Nb_3TeBr_7	52.8	16.0	53.5	18.8
Y_3TeCl_7	18.8	5.6	18.8	6.7
Zr_3TeCl_7	19.3	15.5	19.3	1.9
Mo_3TeCl_7	27.9	52.7	27.8	-12.5
In_3TeCl_7	24.3	10.7	24.1	6.9
Sb_3ICl_7	6.4	14.9	6.4	-4.2
Nd_3TeBr_7	16.8	4.0	16.8	6.2

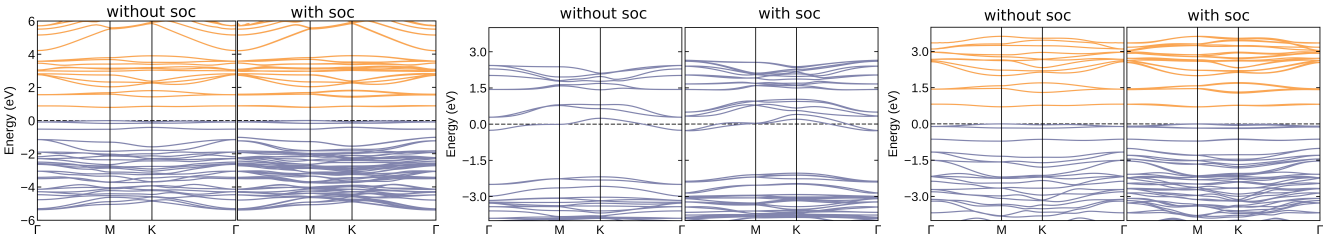

FIG. S2. The band structures of Nb_3SBr_7 (left), Sb_3ICl_7 (middle), and Nb_3TeBr_7 (right) without and with spin-orbit coupling (SOC).

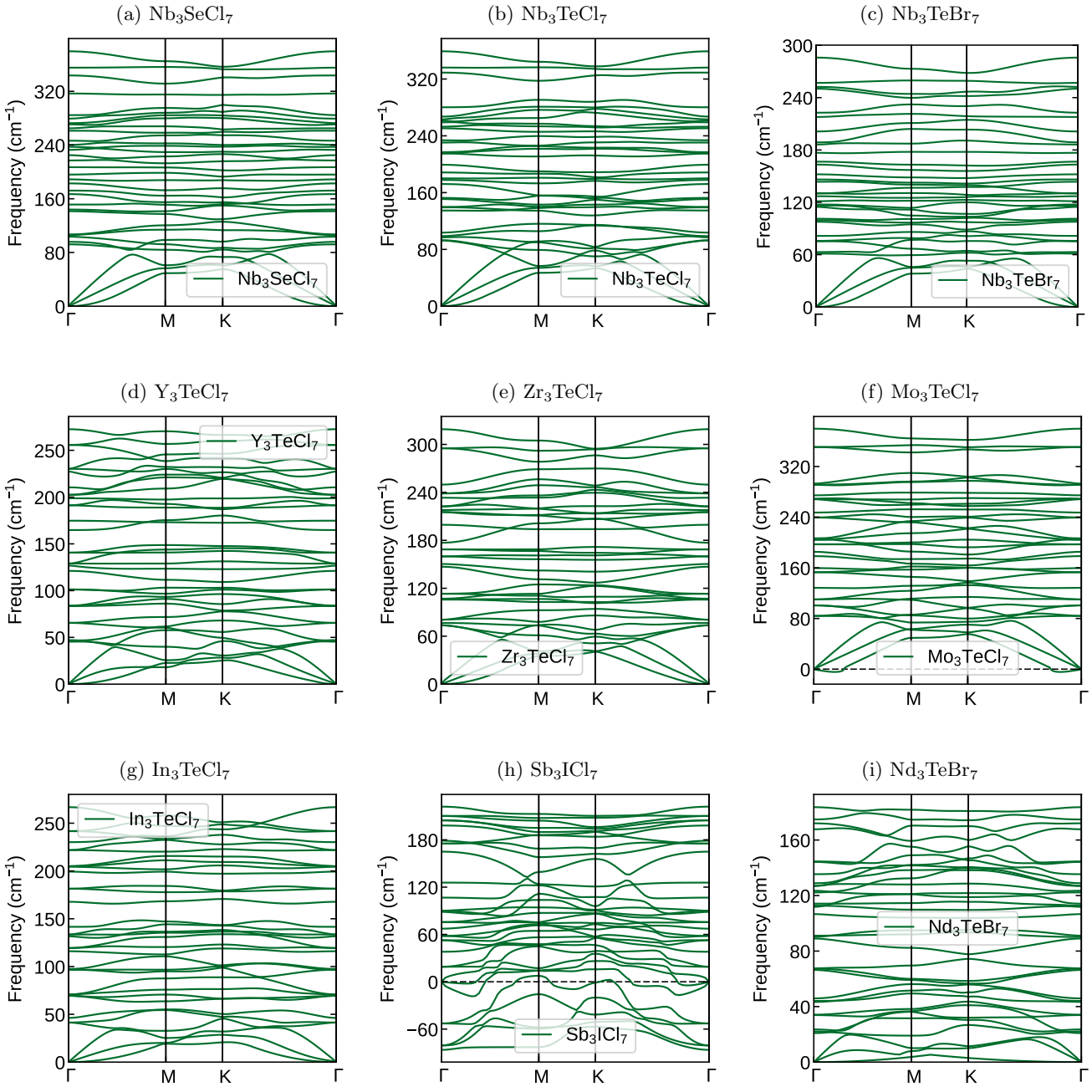

FIG. S3. Phonon band-structure of a few selected members of the M_3QX_7 family.