Supplementary Materials

Physical Properties Investigations of Ternary-Layered Carbides M_2PbC (M = Ti, Zr and Hf): First-Principles Calculations

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Table S1. The equilibrium lattice parameters *a* and *c,* volume *V,* and relaxed atomic parameter Z_M and the formation energy (ΔE_f) for M_2PbC (M= Ti, Zr, Hf) at various pressure conditions.

	Pressure (GPa)	*a* (Å)	*c* (Å)	*c/a*	*V* (Å^3)	Z_M	ΔE_f (eV)
Ti_2PbC	0	3.224	13.926			0.0776	-2.4
	10	3.159	13.574	4.297	117.28	0.0795	-2.354
	20	3.109	13.332	4.288	111.61	0.0807	-2.076
	30	3.064	13.147	4.291	106.90	0.0817	-1.711
	40	3.026	12.992	4.294	103.02	0.0824	-1.289
	50	2.992	12.867	4.300	99.73	0.0830	-0.828
Zr_2PbC	0	3.413	14.868	4.356			
	10	3.334	14.553	4.365	150.02	0.0813	-2.940
	20	3.271	14.317	4.377	140.09	0.9161	-2.783
	30	3.216	14.165	4.405	132.69	0.9147	-2.442
	40	3.167	14.053	4.437	126.89	0.9136	-1.994
	50	3.124	13.960	4.469	122.07	0.9129	-1.472
Hf_2PbC	0	3.386	14.584	4.307	144.80	0.0810	-2.704
	10	3.315	14.265	4.303	135.80	0.0833	-2.56
	20	3.254	14.074	4.325	129.05	0.0846	-2.248
	30	3.203	13.916	4.345	123.66	0.0856	-1.831
	40	3.159	13.798	4.368	119.20	0.0864	-1.348
	50	3.116	13.718	4.402	115.37	0.0871	-0.806

Table S2. The calculated elastic constants, C_{ij} (in GPa), bulk moduli (*B*, in GPa), shear moduli (*G*,in GPa), Young's moduli (*Y*, in GPa), and Poisson's ratio (*v*) for Ti_2PbC, Zr_2PbC and Hf_2PbC at various pressure conditions.

		C_{11}	C_{33}	C_{44}	C_{12}	C_{13}	C_{66}	*B*	*G*	*Y*		*v*
Ti_2PbC	0	244.4	228.2	68.5	100.2	42.4	72.1	119.8	76.2	188.6	0.707	0.238
	10	310.1	317.2	105.7	113.8	82.3	98.2	165.9	105.5	261.1	0.914	0.238
	20	377.2	394.5	138.7	133.1	111.1	122.1	206.9	132.4	327.4	1.020	0.236
	30	438.2	457.2	169.4	150.7	136.5	143.7	242.3	156.7	386.7	1.089	0.234
	40	495.9	524.6	200.2	168.5	163.5	163.7	278.5	180.1	444.5	1.155	0.234
	50	572.21	609.8	228.2	204.3	165.6	183.9	313.9	208.2	511.5	1.073	0.228
Zr_2PbC	0	220.11	219.9	69.8	68.5	62.9	76.2	116.3	74.1	183.4	0.889	0.237

	10	287.11	298.4	105.7	82.3	98.4	102.7	158.5	102.4	252.8	1.088	0.234
	20	347.1	367.6	136.8	94.9	129.2	126.6	195.8	126.8	312.9	1.199	0.234
	30	421.8	428.8	157.5	122.8	140.9	161.4	231.5	152.7	375.5	1.106	0.230
	40	465.4	510.1	195.5	130.8	194.0	165.8	273.8	171.1	424.8	1.331	0.241
	50	507.1	537.1	192.9	147.2	201.1	182.2	293.6	179.6	447.5	1.202	0.246
Hf_2PbC	0	286.8	263.2	88.1	65.4	77.4	110.7	141.6	98.1	239.1	0.892	0.219
	10	357.0	336.1	127.8	88.2	107.1	134.4	183.8	127.5	310.7	1.067	0.219
	20	420.0	407.3	162.1	111.8	129.9	154.1	221.4	153.7	374.5	1.143	0.218
	30	473.0	458.4	181.6	143.5	149.4	174.3	254.1	171.0	419.0	1.148	0.225
	40	500.3	512.2	207.8	142.9	181.2	178.7	280.1	184.8	454.5	1.279	0.230
	50	542.8	561.4	232.7	155.9	202.1	193.6	307.1	202.6	498.2	1.323	0.230

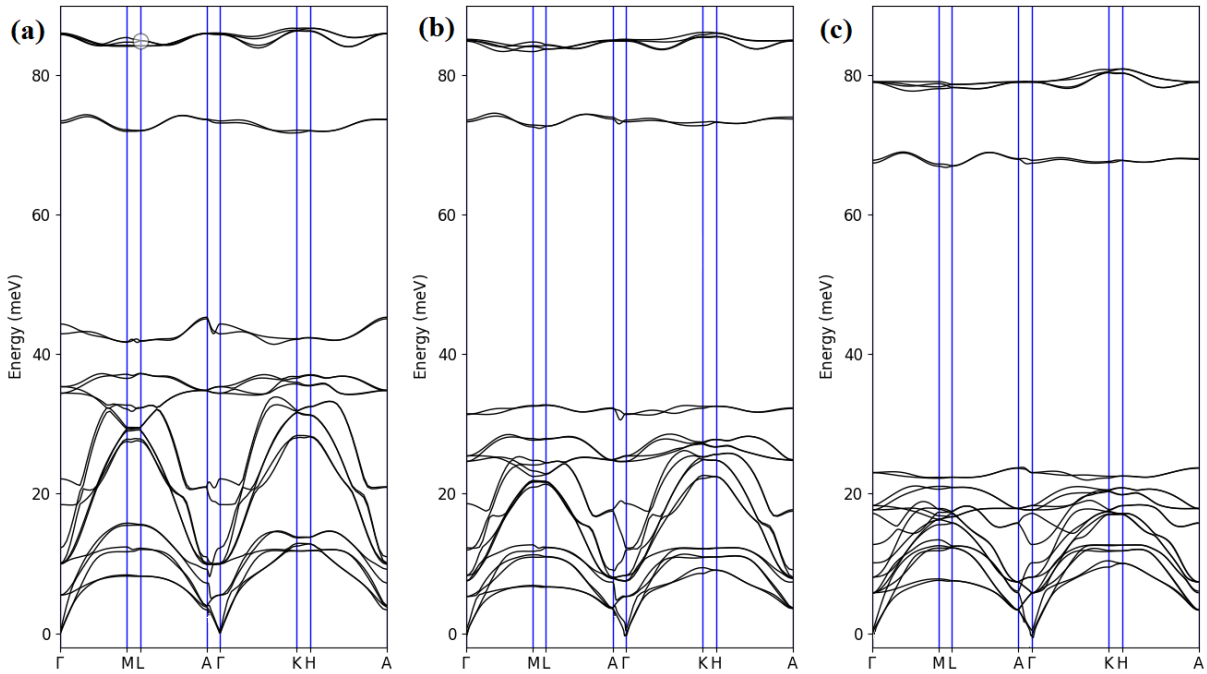

Figure S1. Phonon band dispersion curves of the M_2PbC MAX phase (M =Ti, Zr, Hf),

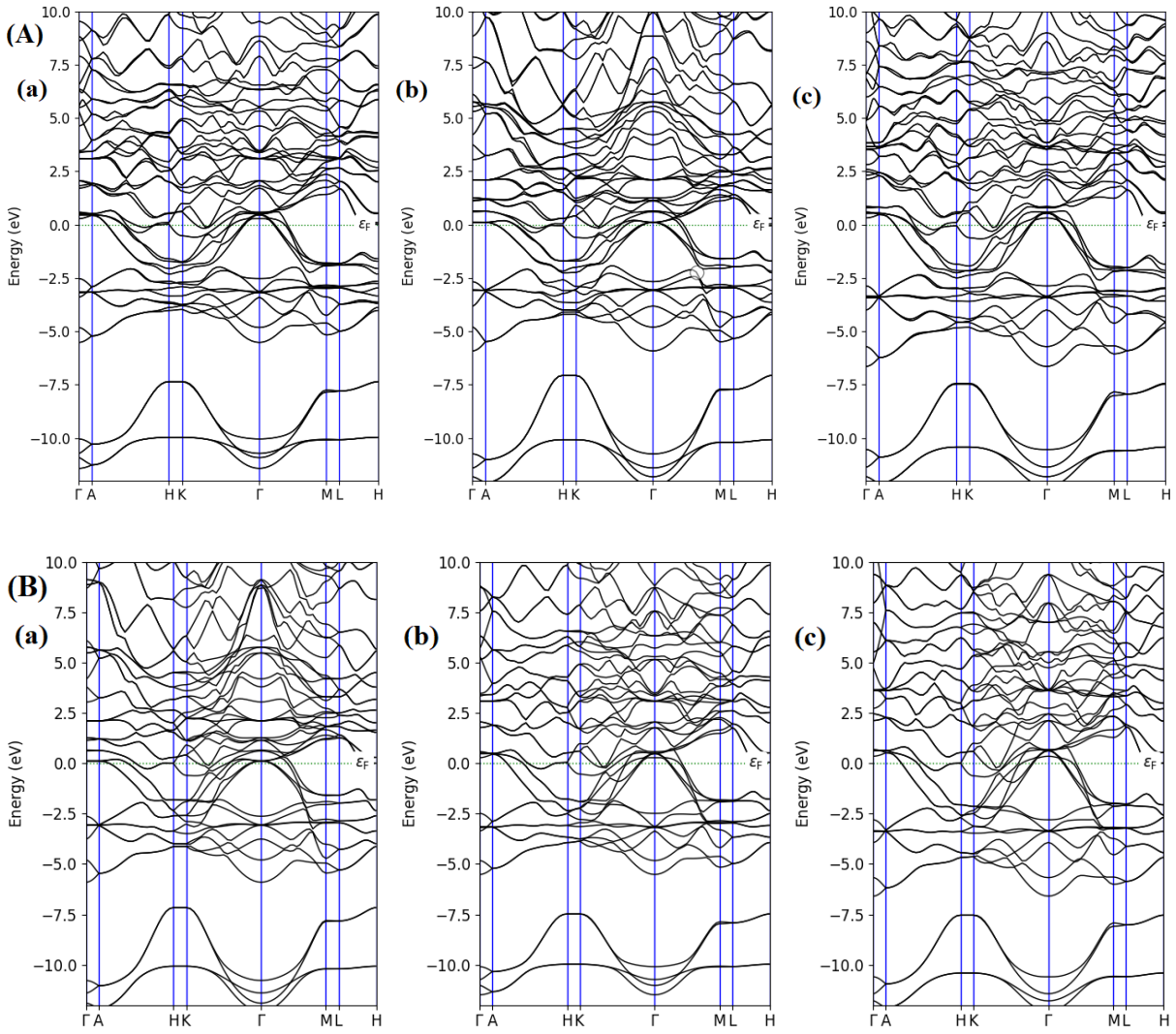

Figure S2. Electronic band structure of (a) Ti_2PbC, (b) Zr_2PbC, and (c) Hf_2SnC (A) with and (B) without SOC contribution