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A first-principles investigation of a new hard multi-layers MnB_2 structure

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Table S1. Calculated elastic constants C_{ij} (GPa) for *Immm*-MnB_2 and some common transition metal diborides TMB_2(TM= Ta, W, Re) at P= 0 or 50 GPa.

Structure	P	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
Immm-MnB_2	0	653	442	643	273	161	166	178	170	189
	50	910	673	899	374	239	231	242	240	312
*P*6/*mmm*-TaB_2	0	605		475	233		225	154	206	
	0									
	0	598[a]		442[a]	208[a]		227[a]	145[a]	214[a]	
$P6_3/mmc$-WB_2	0	550		650	225		188	173	221	
	0	571[b]		672[b]	202[b]		213[b]	145[b]	200[b]	
$P6_3/mmc$-ReB_2	0	626		1045	263		223	180	122	
	0	643[c]		1035[c]	263[c]		244[c]	159[c]	129[c]	
	0	675[d]		1081[d]	278[d]		264[d]	147[d]	115[d]	

[a] Ref 42, [b] Ref 43, [c] Ref 44, [d] Ref 16

Fig. S1. The calculated energy versus volume curves for *Immm*-MnB_2 using non-spin-polarized and spin-polarized calculations.

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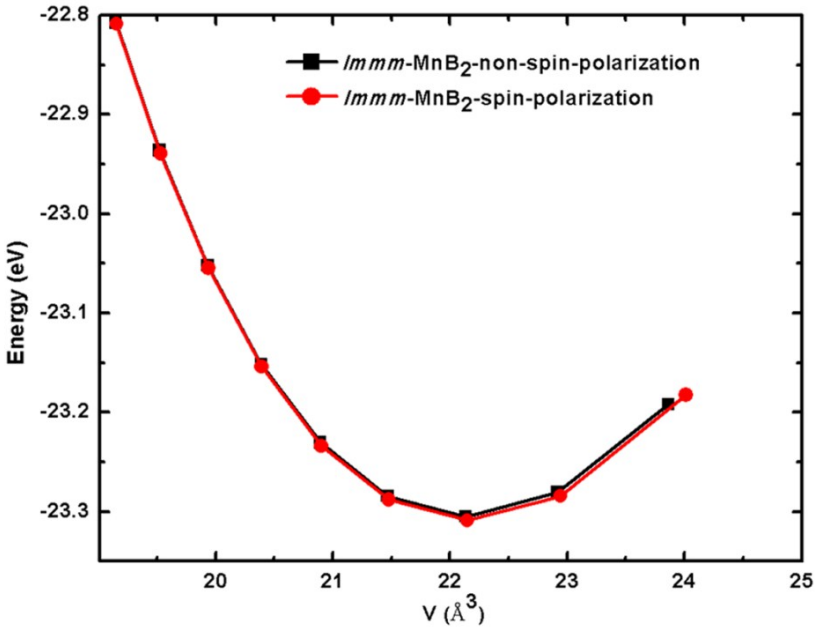

Fig. S2. Magnetic moment versus pressure for *Immm*-MnB_2 using spin-polarized calculation.

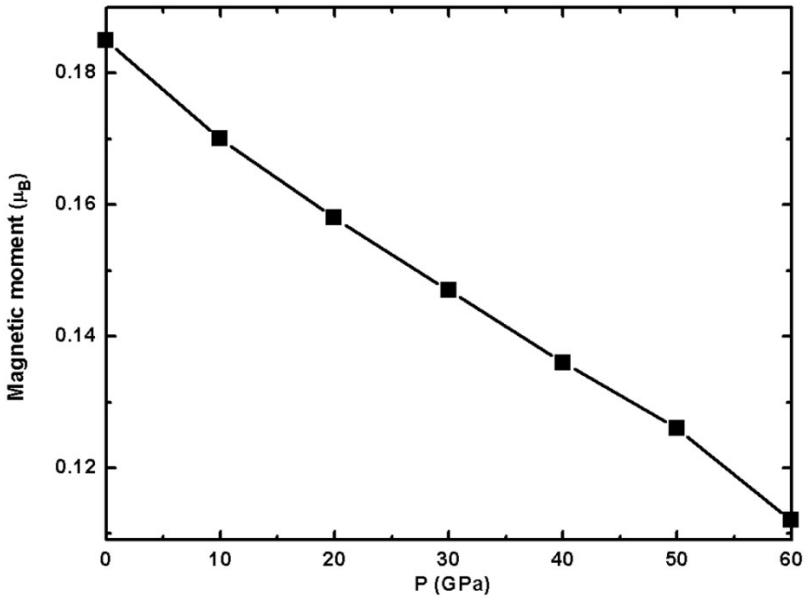

Table S2. Bader charge analysis for *Immm*-MnB_2 at 0 GPa.

Immm-MnB_2		
Atom	Charge value (e)	δ(e)
Mn	12.36	0.64
Mn	12.36	0.64
Mn	12.52	0.48
Mn	12.52	0.48
Mn	12.52	0.48
Mn	12.52	0.48
B	3.42	-0.42
B	3.45	-0.45
B	3.42	-0.42
B	3.45	-0.45
B	3.20	-0.20
B	3.16	-0.16
B	3.20	-0.20
B	3.16	-0.16
B	3.20	-0.20
B	3.16	-0.16
B	3.20	-0.20
B	3.16	-0.16