Pressure-induced Structural Phase Transition and Thermoelectric Properties of Bulk Mg_3Bi_2

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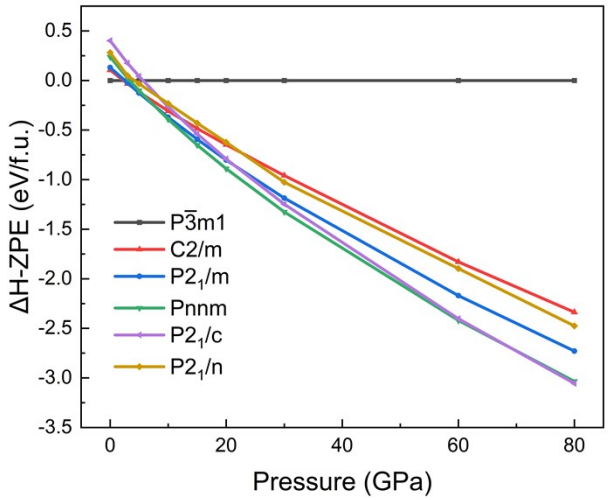

Fig. S1 Calculated enthalpy curves as a function of pressure for each phase of Mg_3Bi_2, including zero-point energy (ZPE) correction.

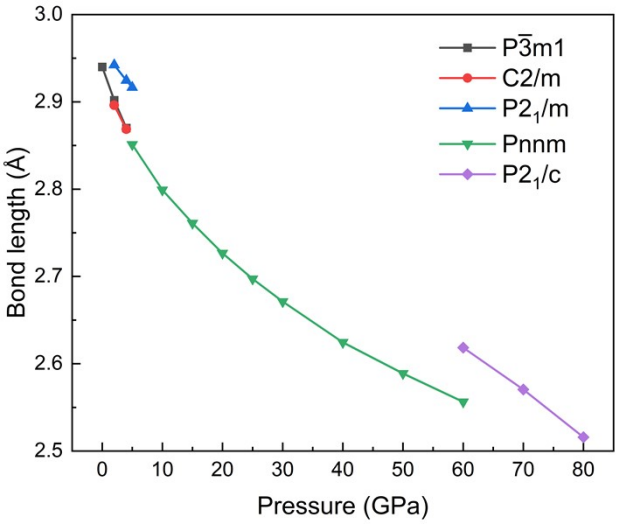

Fig. S2 Nearest-neighbor Mg-Bi bond lengths in different phases of Mg_3Bi_2.

Table SI. Calculated Bader charge analysis for the $P\bar{3}m1$, $P2_1/m$, *Pnnm,* and $P2_1/c$ phases at 0, 4, 30, and 80 GPa, respectively. δ denotes the number of electrons transferred per atom.

Space Group	Atom	Charge value (*e*)	δ (e)
$P\bar{3}m1$	Mg	1.6444	-0.3556
	Bi	15.5334	0.5334
$P2_1/m$	Mg	1.57605	-0.42396
	Bi	15.63593	0.63593
Pnnm	Mg	1.41377	-0.58623
	Bi	15.87934	0.87934
$P2_1/c$	Mg	2.28363	0.28363
	Bi	14.57456	-0.42544

Table SII. Calculated elastic constants *C*ij (in GPa) for the $P2_1$/m, *Pnnm,* and $P2_1$/c phases at 4, 30, and 80 GPa, respectively.

Space Group	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	
	C_{12}	C_{13}	C_{15}	C_{23}	C_{25}	C_{35}	C_{46}
$P2_1$/m	85.9562	84.2405	64.8930	23.2191	15.2180	15.3035	
	38.5359	37.8527	-1.8620	45.6931	2.4922	5.1985	-6.4511
Pnnm	225.9996	208.4193	219.5799	61.2096	35.3170	4.8001	
	102.7286	121.5137	0.0000	123.4532	0.0000	0.0000	0.0000
$P2_1$/c	501.3339	442.0004	450.3864	72.3231	46.8994	33.9619	
	230.8434	205.0906	18.3408	271.3051	-13.9276	-11.4988	-4.8967