Supporting Information

Pressure induced semiconductor-semimetal-superconductor transition for magnesium hexaborides

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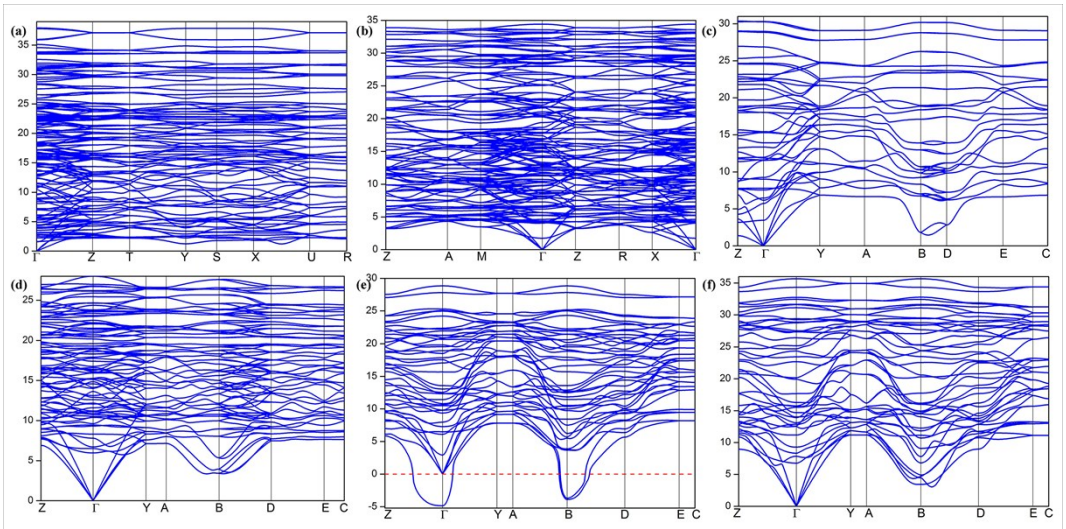

Fig. S1 Phonon dispersion curves of (a) *Cmcm*, (b) *I*4/*mmm*, (c) *C*2/*m*-I, (d) *C*2/*m*-II and (e) $P2_1/m$ at zero pressure, (f) $P2_1/m$ at 70GPa for MgB_6.

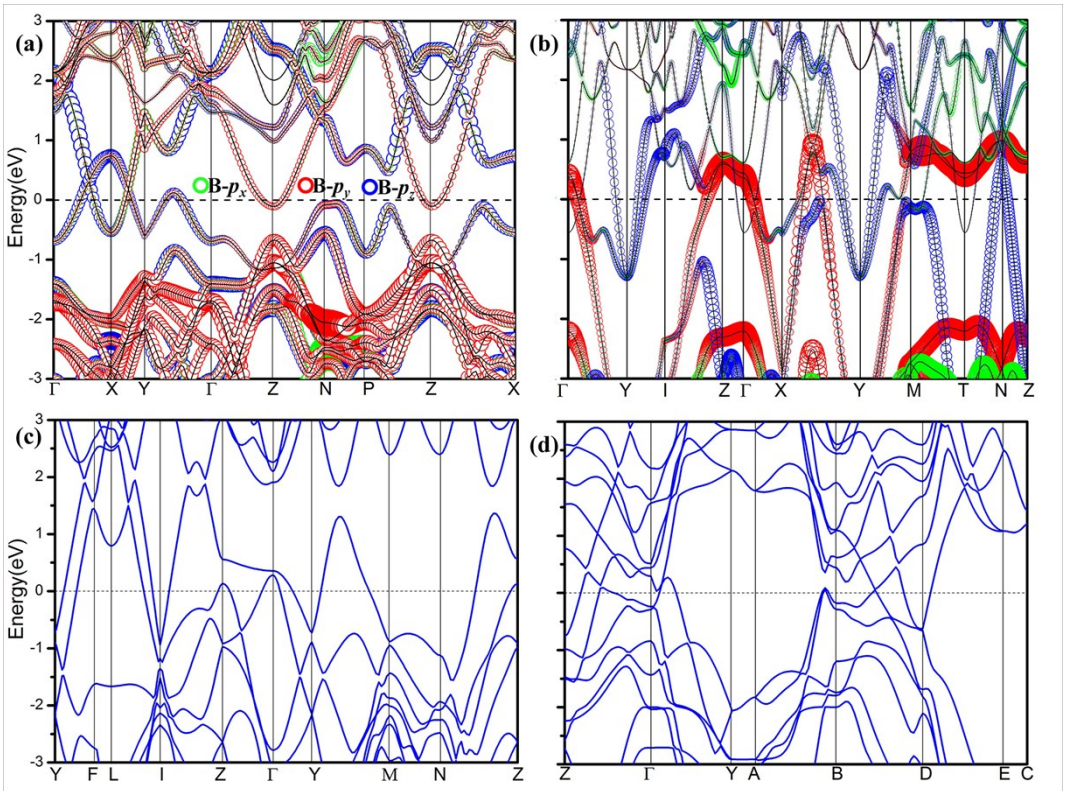

Fig. S2 Bands structure of (a) *I*4/*mmm*, (b) *C*2/*m*-I, (c) *C*2/*m*-II, (d) $P2_1/m$ of MgB_6.

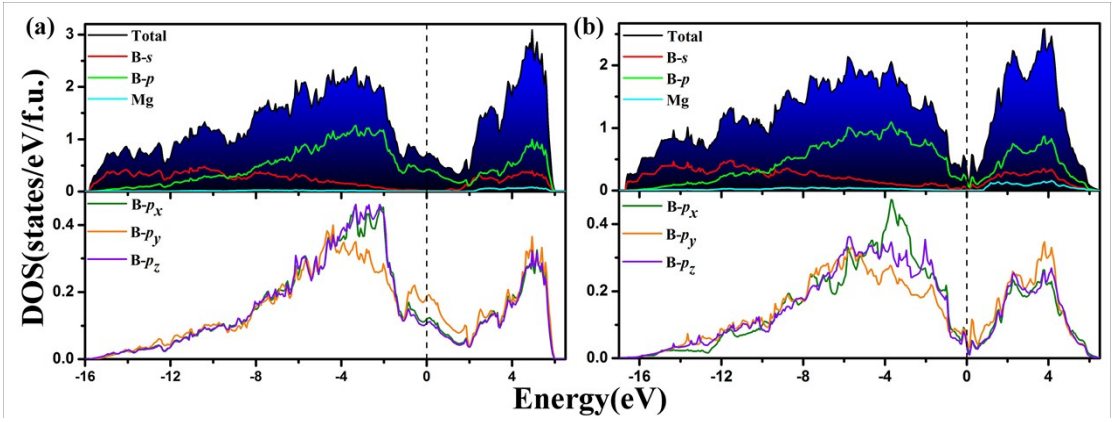

Fig. S3 The densities of states calculated by PBE (a) *C*2/*m*-II, (b) $P2_1$/m at ambient pressure.

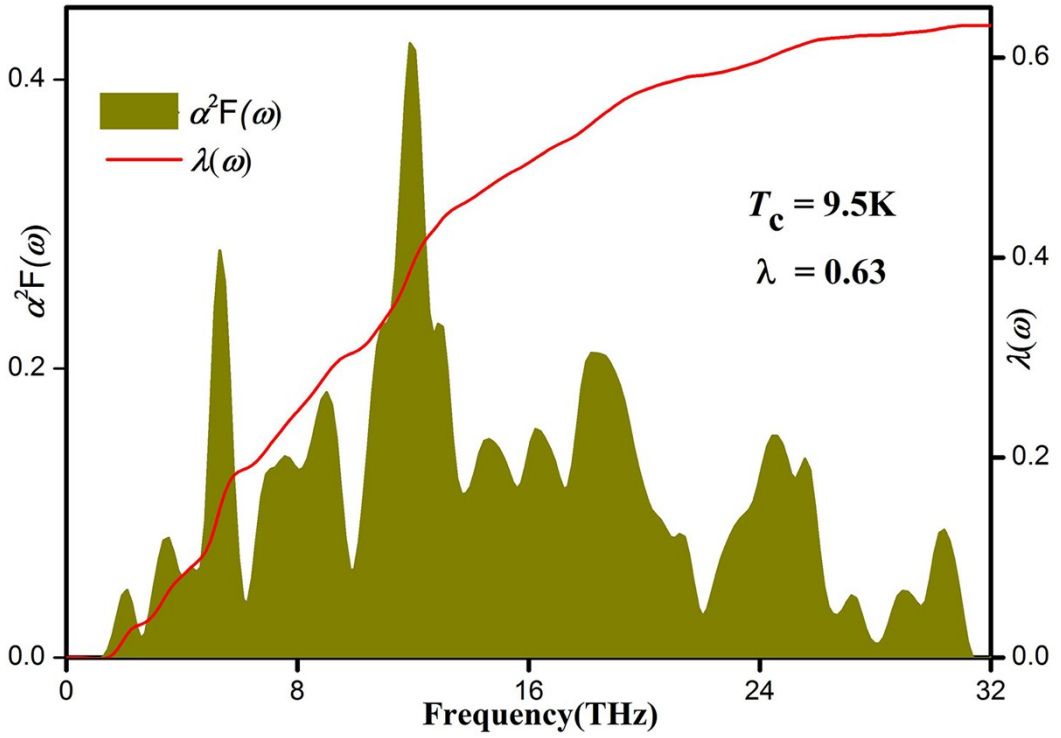

Fig. S4 Eliashberg spectral function $\alpha^2F(\omega)$ (dark yellow area) and electron-phonon coupling parameters $\lambda(\omega)$ (red line) of *C*2/*m*-I for MgB_6.

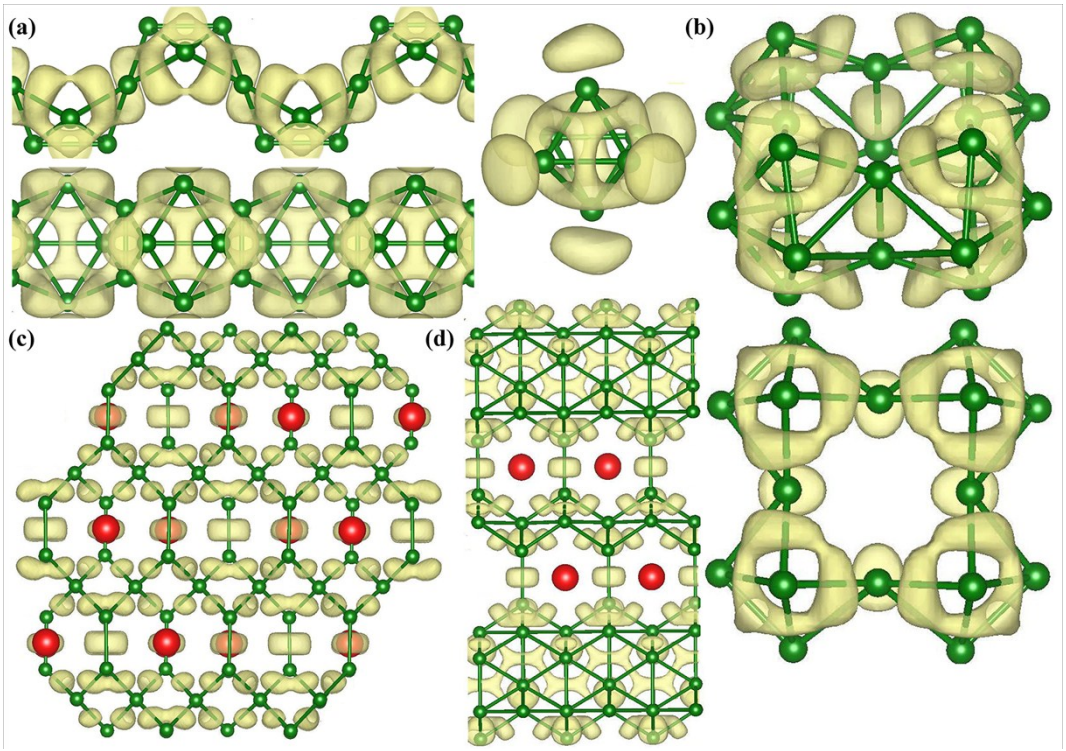

Fig. S5 The ELF with isosurfaces 0.75 (a) B_8 cluster and B_6 octahedra of *Cmcm* structure, (b) B_{24} cluster of *I*4/*mmm* structure, (c) *C*2/*m*-II, (d) $P2_1/m$.

Born-Huang criteria for

orthorhombic phase:

$C_{ii}>0(i=1\sim6)$,

$(C_{11}+C_{22}-2C_{12})>0$, $(C_{11}+C_{33}-2C_{13})>0$, $(C_{22}+C_{33}-2C_{23})>0$,

$[C_{11}+C_{22}+C_{33}+2(C_{12}+C_{13}+C_{23})]>0$.

tetragonal phase:

$C_{ii}>0$ (i=3, 4, 6),

$C_{11}-C_{12}>0$,

$C_{11}+C_{33}-2C_{13}>0$,

$2C_{11}+C_{33}+2C_{12}+4C_{13}>0$.

monocilnic structure:

$C_{ii}>0$ (i= 1, 2, 3, 4, 5, 6),

$[C_{11}+C_{22}+C_{33}+2(C_{12}+C_{13}+C_{23})]>0$,

$(C_{33}C_{55}-C_{35}^2)>0$, $(C_{44}C_{66}-C_{46}^2)>0$, $(C_{22}+C_{33}-2C_{23})>0$,

$[C_{22}(C_{33}C_{55}-C_{35}^2)+2C_{23}C_{25}C_{35}-C_{23}^2C_{55}-C_{25}^2C_{33}]>0$,

$\{2[aC_{15}C_{25}+bC_{15}C_{35}+cC_{25}C_{35}]-[dC_{15}^2+eC_{25}^2+fC_{35}^2]\}+gC_{55}>0$,

$a=C_{33}C_{12}-C_{13}C_{23}$, $b=C_{22}C_{13}-C_{12}C_{23}$, $c=C_{11}C_{23}-C_{12}C_{13}$,

$d=C_{22}C_{33}-C_{23}^2$, $e=C_{11}C_{33}-C_{13}^2$, $f=C_{11}C_{22}-C_{12}^2$,

$g=C_{11}C_{22}C_{33}-C_{11}C_{23}^2-C_{22}C_{13}^2-C_{33}C_{12}^2+2C_{12}C_{13}C_{23}$.

Table S1. The Wyckoff positions of the proposed MgB_6 structures are listed.

	atoms	x	y	z	site
Cmcm	Mg	-0.29123	-0.63821	0.75000	8*g*
	B1	-0.35423	-0.35694	0.75000	8*g*
	B2	0.16798	-0.42073	0.75000	8*g*
	B3	-0.00000	-0.64058	1.41019	8*f*
	B4	0.00000	-0.93983	-0.93983	8*f*
	B5	-0.00000	-0.22821	1.09012	8*f*
	B6	-0.09786	-0.50000	0.50000	8*e*
*I*4/*mmm*	Mg1	0.00000	0.00000	0.81648	4*e*
	Mg2	-0.00000	0.50000	0.25000	4*d*
	B1	0.28091	0.50000	0.08942	16*n*
	B2	0.27527	0.27527	0.16088	16*m*
	B3	0.12371	0.70010	-0.00000	16*l*
*C*2/*m*-I	Mg	-0.50000	-0.00000	-0.00000	2*b*
	B1	0.52215	-0.50000	0.27674	4*i*
	B2	0.66639	-0.00000	0.73943	4*i*
	B3	0.65047	-0.00000	0.49065	4*i*
*C*2/*m*-II	Mg	-0.33501	-0.00000	0.82714	4*i*
	B1	-0.66187	-0.25878	0.67179	8*j*
	B2	-0.12456	0.00000	0.02290	4*i*
	B3	-0.20420	-0.00000	0.32761	4*i*
	B4	-0.53754	-0.00000	0.65646	4*i*
	B5	-0.50000	0.25921	-0.00000	4*g*
$P2_1/m$	Mg	-0.68671	-0.25000	1.15591	2*e*
	B1	-0.22485	-0.25000	0.34295	2*e*
	B2	-0.49698	-0.25000	0.79945	2*e*
	B3	-0.40498	-0.25000	1.33352	2*e*
	B4	-0.13181	-0.75000	0.48382	2*e*
	B5	-0.04557	-0.75000	1.04339	2*e*
	B6	-0.86741	-0.75000	1.13269	2*e*

Table S2. The elastic constants C_{ij} (GPa), bulk moduli B (GPa), the shear moduli G (GPa), Young's modulus E (GPa), the B/G value and Poisson ratio v for the $C2/m$-II and $P2_1/m$ of MgB_6.

	$C2/m$-II	$P2_1/m$(70 GPa)
C_{11}	478	771
C_{22}	371	757
C_{33}	458	753
C_{44}	229	262
C_{55}	188	344
C_{66}	230	260
C_{12}	136	200
C_{13}	67	193
C_{15}	-39	44
C_{23}	118	152
C_{25}	69	-48
C_{35}	-39	57
C_{46}	32	-18
B	213	
G	179	
E	420	
B/G	1.19	
v	0.171	