Supplemental Material for

Iron-magnesium compounds under Earth's inner core conditions

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Table S1. Structure information of the Fe-Mg compounds at selected pressures. Atomic positions are in fractional coordinates. Lattice parameters are in units of Å.

Structure	Lattice Parameters	Atom	Atomic positions		
***I*4/*mmm*-Fe_2Mg (360GPa)	a = 2.32 c = 7.29	Fe	0.50	0.50	0.67
		Mg	0.00	0.00	0.50
***R*-3*m*-$FeMg_4$ (360GPa)	a = 3.38 c = 10.47	Fe	0.00	0.00	0.00
		Mg	0.00	0.00	0.20
		Mg	0.00	0.00	0.40
***Fm*-3*m*-$FeMg_3$ (360GPa)	a = 4.78	Fe	0.00	0.50	0.50
		Mg	0.25	0.25	0.25
		Mg	0.00	0.50	0.00
***P*63/*mmc*-$FeMg_2$ (360GPa)	a = 3.40 c = 4.00	Fe	0.33	0.67	0.75
		Mg	0.00	0.00	0.00
		Mg	0.33	0.67	0.25
***Fd*-3*m*-FeMg (360GPa)	a = 4.73	Fe	0.00	0.50	0.00
		Mg	0.50	0.50	0.00
***R*-3*m*-Fe_2Mg_3 (360GPa)	a = 3.36 c= 20.61	Fe	0.00	0.00	0.35
		Fe	0.00	0.00	0.55
		Mg	0.00	0.00	0.75
		Mg	0.00	0.00	0.15

		Mg	0.00	0.00	0.05
***Pmmn*-$FeMg_3$ (200GPa)**	*a*= 3.71	Fe	0.00	0.00	0.35
	b= 4.44	Mg	0.00	0.50	0.36
	c= 4.11	Mg	0.50	0.75	0.15
***Cmcm*-$FeMg_2$ (200GPa)**	*a*=3.67	Fe	0.50	0.07	0.25
	b= 7.69	Mg	0.00	0.09	0.75
	c= 3.56	Mg	0.50	0.25	0.75
***P*4_132-Fe_2Mg_3 (100GPa)**	*a* = 5.79	Fe	0.18	0.82	0.32
		Mg	0.38	0.79	0.96

Table S2. Calculated Bader partial charges normalized by the total charges at 360GPa.

Structure	Atom	Partial charge
***I*4/*mmm*-Fe_2Mg**	Fe	+0.7
	Mg	-1.4
***R*-3*m*-$FeMg_4$**	Fe	+5.5
	Mg	-1.4
***Fm*-3*m*-$FeMg_3$**	Fe	+4.0
	Mg	-1.3
***P*63/*mmc*-$FeMg_2$**	Fe	+2.7

	Mg	-1.4
***R*-3*m*- Fe_2Mg_3**	Fe1	+1.4
	Fe2	+2.6
	Mg	-1.4
***Fd*-3*m*-FeMg**	Fe	+1.4
	Mg	-1.4

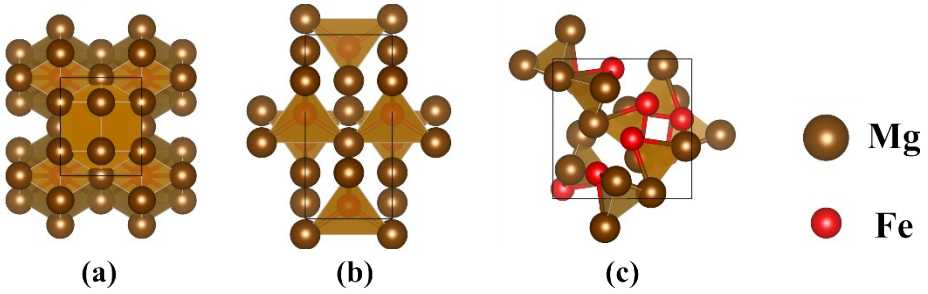

Figure S1. Predicted stable crystal structures of *Pmmn*-$FeMg_3$ (a), *Cmcm*-$FeMg_2$ (b) and $P4_132$-Fe_2Mg_3 (c).

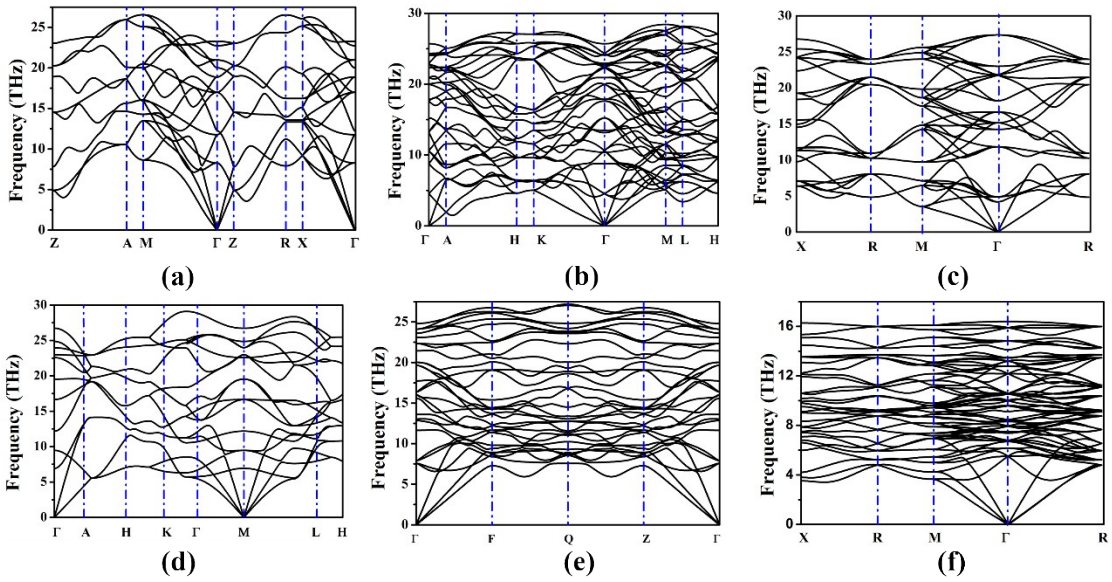

Figure S2. Calculated phonon band structure for *I*4/*mmm*-Fe_2Mg (a), *R*-3*m*-$FeMg_4$ (b), *Fm*-3*m*-$FeMg_3$ (c), *P*63/*mmc*-$FeMg_2$ (d), *R*-3*m*-Fe_2Mg_3 (e) and *Fm*-3*m*-FeMg (f) at 360GPa, respectively.

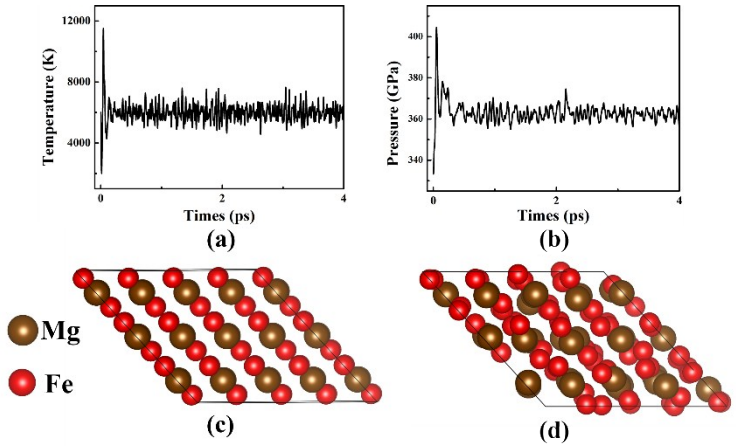

Figure S3. Temperature (a) and pressure (b) as a function of MD time in NVT simulation for *I*4/*mmm*-Fe_2Mg. Structures for *I*4/*mmm*-Fe_2Mg at 0 ps (c) and 4 ps (d), respectively. The 3×3×4 supercell of 108 atoms for the primitive cell was employed.

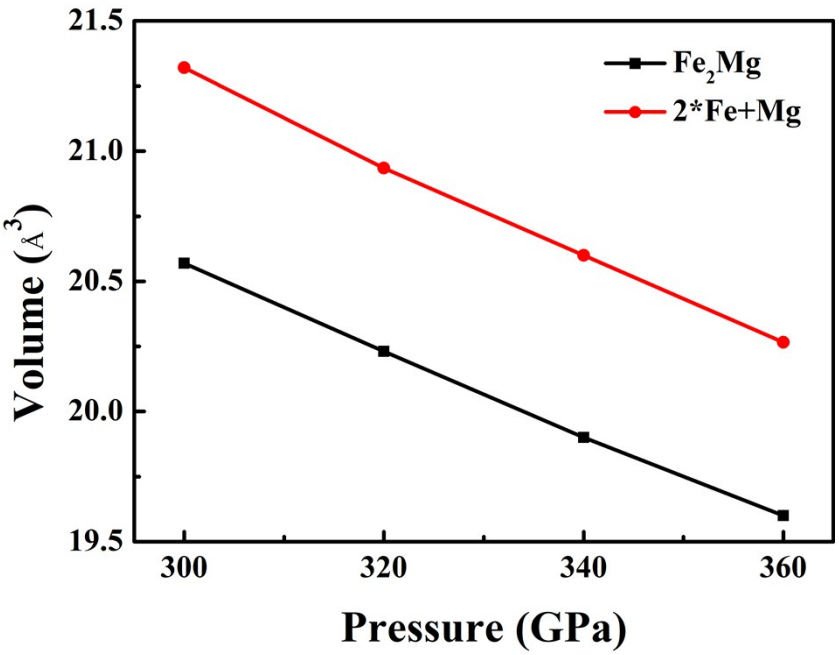

Figure S4. Theoretical pressure dependency of the volume/f.u. for Fe_2Mg (black line) and the sum of volume/atom for hcp Fe and bcc Mg (red line). The volume of Fe_2Mg is smaller than the sum of Fe and Mg under pressure, revealing that pressure help the mix of Fe and Mg.