Supporting Information

Structure searching and phase relations in MnN up to 50 GPa: a DFT study

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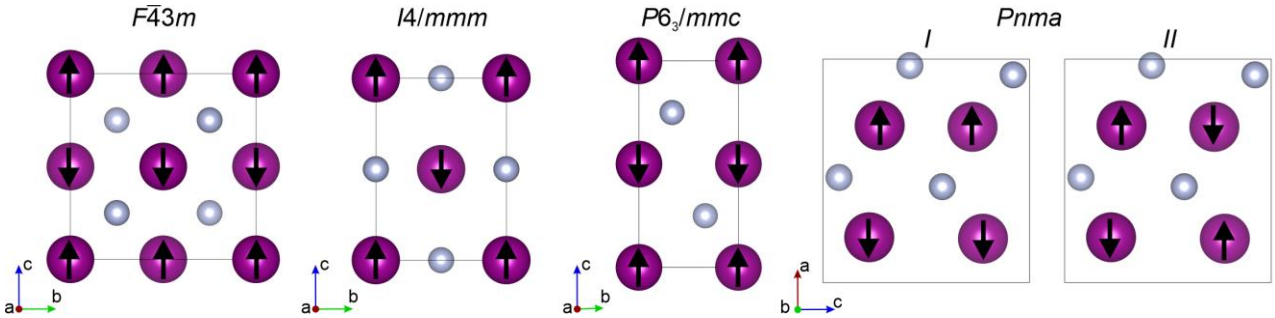

Figure S1. The considered initial antiferromagnetic configurations for the predicted MnN polymorphs.

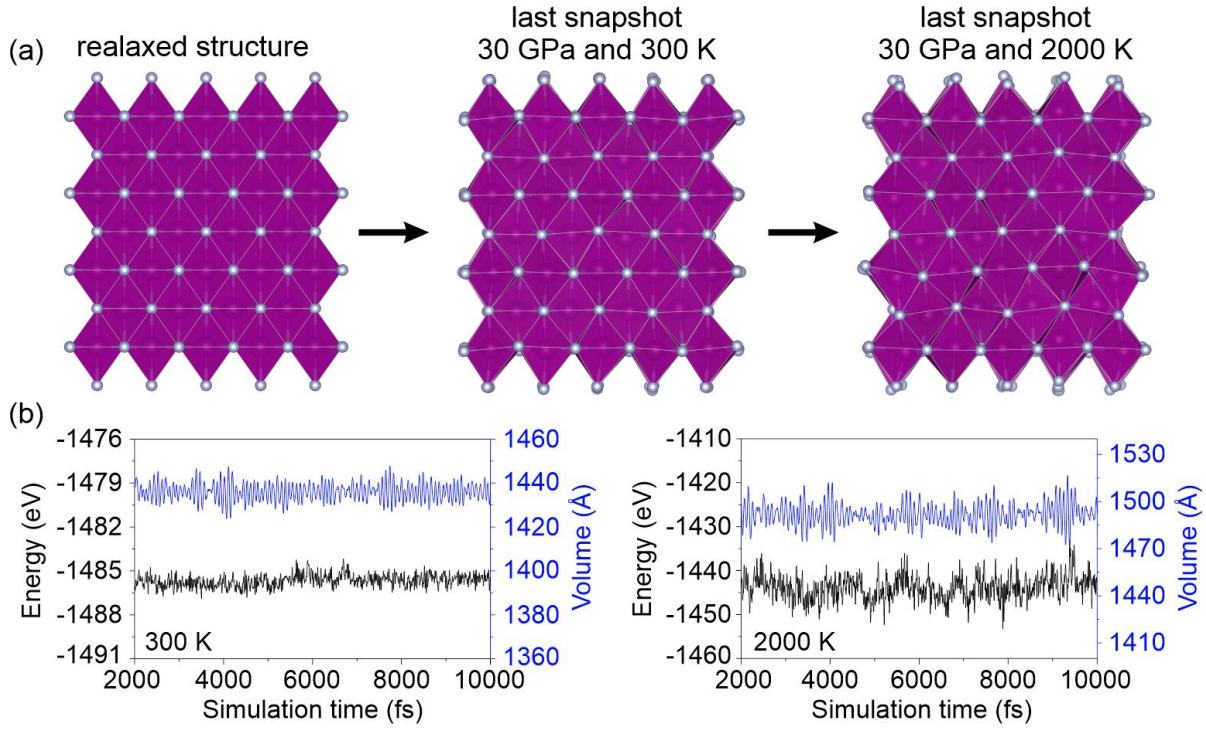

Figure S2. (a) The relaxed structure of MnN-*I*4/*mcm* and the last snapshots from the MD simulations at 30 GPa and 300 and 2000 K. (b) Calculated energy and volume as a function of simulation time at 30 GPa and 300 and 2000 K.

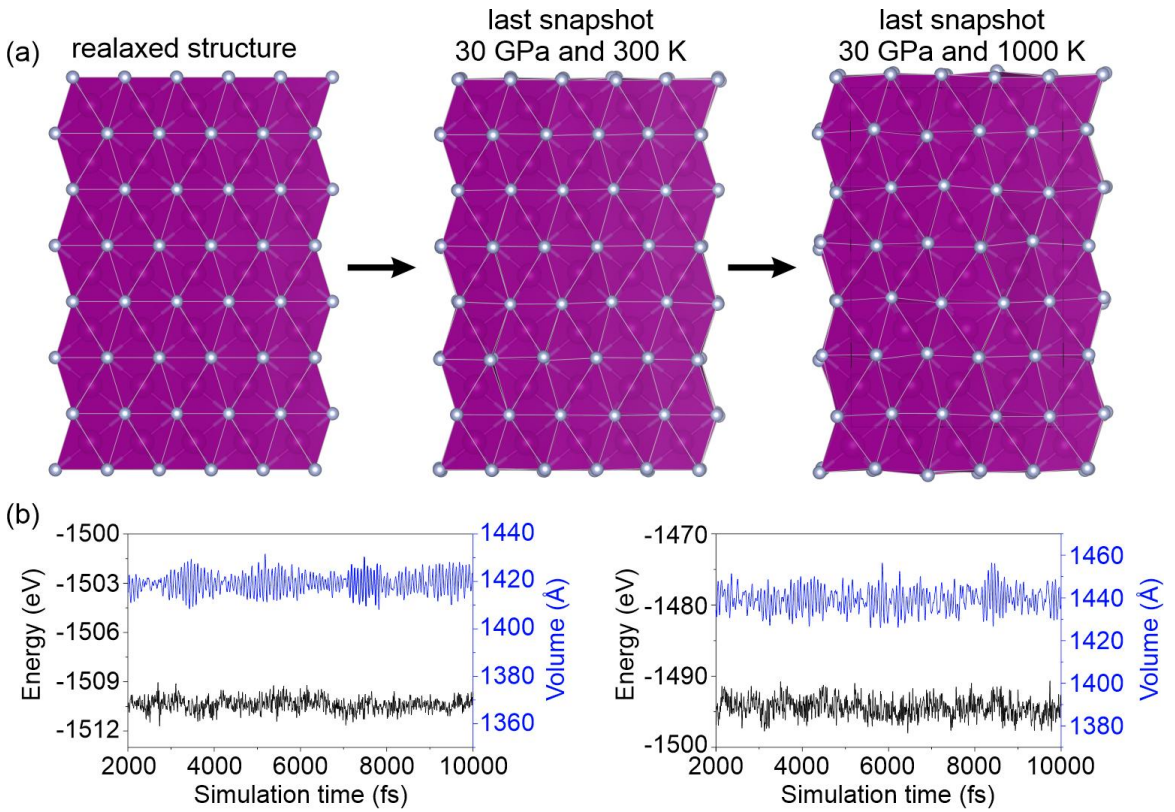

Figure S3. (a) The relaxed structure of MnN-$P6_3/mmc$ and the last snapshots from the MD simulations at 30 GPa and 300 and 1000 K. (b) Calculated energy and volume as a function of simulation time at 30 GPa and 300 and 2000 K.

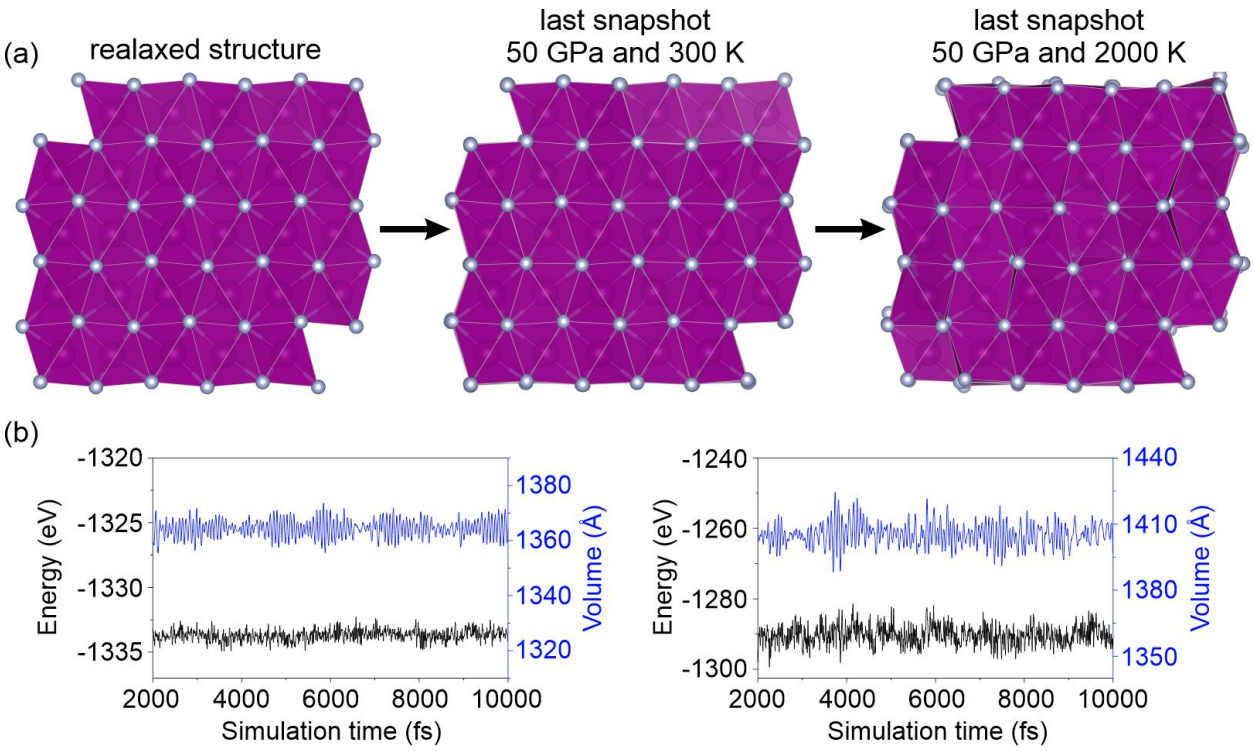

Figure S4. (a) The relaxed structure of MnN-*Pnma* and the last snapshots from the MD simulations at 50 GPa and 300 and 2000 K. (b) Calculated energy and volume as a function of simulation time at 30 GPa and 300 and 2000 K.

Table S1. Calculated enthalpies of MnN polymorphs with U_{eff} = 3.9 eV at 58 GPa. Relative enthalpies ΔH are normalized to the enthalpy of $P6_3/mmc$.

Polymorph	Magnetic state	Enthalpy (eV/f.u.)	ΔH (eV/f.u.)
$P6_3$/mmc	*afm*	-8.74027	0.07111
	fm	-8.81138	0
	nm	-7.82395	0.98743
Pnma	*fm*	-8.81088	0.00050
	nm	-7.82699	0.98439
*I*4/*mmm*	*afm*	-8.74027	0.07111
	nm	-7.82395	0.98743
$Fm\bar{3}m$	*fm*	-9.08220	-0.27081
	nm	-7.09535	1.71603
$F\bar{4}3m$	*afm*	-7.51206	1.29932
	fm	-7.41699	1.39439
	nm	-6.87959	1.93179

*It is worth noting that the study of phase relations using the DFT+U method is invalid, since for each polymorph it is necessary to select its own parameter U_{eff} and the energies obtained with different U cannot be compared (as mentioned in the VASP manual). Here we perform DFT+U calculations just to show the invalidity of the obtained enthalpy relations with U correction.

Table S2. Calculated elastic constants C_{ij} (in GPa) of MnN polymorphs at various pressures (GPa).

Phase	Pressure	C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
*I*4/*mmm*	0	164.2	56.2	46.1	164.2	46.1	170.6	42.3	42.3	48.1
	10	424.6	159.4	108.6	423.9	108.6	448	103.6	103.6	132.5
	20	487.1	220.3	146.1	487	146.1	591.6	100.2	100.2	194
	30	541.9	274.6	149.7	542.2	149.7	703.7	95.4	95.4	238.8
	40	577.2	307.9	163.6	577.6	163.6	789.2	87.6	87.6	259.6
$F\bar{4}3m$	0	303.3	207.6	207.6	303.3	207.6	303.3	31.2	31.2	31.2
	5	300.9	220.3	220.3	300.9	220.3	300.9	14.1	14.1	14.1
$P6_3/mmc$	5	458.6	167.0	148.3	461.7	148.3	668.0	157.3	157.3	146.0
	10	479.0	187.4	168.2	483.4	168.2	705.1	172.8	172.8	146.9
	20	513.0	221.9	209.6	520.1	209.6	791.1	201.4	201.4	148.7
	30	505.4	255	247.6	527.8	247.6	873.6	228.7	228.7	143.0
	40	375.5	218.7	429.4	366.4	429.4	940.4	251.7	251.8	97.0
Pnma	40	906.1	421.3	480.7	660.6	300.1	661.6	194.7	260.0	281.8
	50	986.1	437.7	499.3	780.0	382.4	788.1	203.2	280.0	304.5

The Born stability criteria

For cubic crystals:

$$C_{11} > 0, \quad C_{44} > 0, \quad C_{11} > |C_{12}|, \quad (C_{11} + 2C_{12}) > 0$$

For hexagonal crystals:

$$C_{44} > 0, \quad C_{11} > |C_{12}|, \quad (C_{11} + 2C_{12})C_{33} - 2C_{13}^2 > 0$$

For tetragonal crystals:

$$C_{11} > 0, \quad C_{33} > 0, \quad C_{44} > 0, \quad C_{66} > 0,$$
$$(C_{11} - C_{12}) > 0, \quad (C_{11} + C_{33} - 2C_{13}) > 0\,, \quad [2(C_{11} + C_{12}) + C_{33} + 4C_{13}] > 0$$

For orthorhombic crystals:

$$C_{11} > 0, \quad C_{22} > 0, \quad C_{33} > 0, \quad C_{44} > 0, \quad C_{55} > 0, \quad C_{66} > 0,$$
$$[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] > 0, \quad (C_{11} + C_{22} - 2C_{12}) > 0\,,$$
$$(C_{11} + C_{33} - 2C_{13}) > 0, \quad (C_{22} + C_{33} - 2C_{23}) > 0$$