Electronic Supplementary Material

Scanning the latent phases and superconductivity in the Nb-Pb system at high pressure

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Table S1 The relative total energies of several Nb_3Pb (at 0 GPa) compounds.

Space Group	OQMD-ID[a]	relative total energies (meV/atom)
Pmn (A15)[b]	17740	7.68527
P63/mmc	318944	68.17163
Pmm	343430	76.01067
I4/mmm	298645	149.0937
Fmm	309183	177.5072

a: ID from The Open Quantum Materials Database (OQMD), Saal, J. E., Kirklin, S., Aykol, M., Meredig, B., and Wolverton, C. "Materials Design and Discovery with High-Throughput Density
b: https://materials.springer.com/isp/crystallographic/docs/sd_0251819, Dataset ID:sd_0251810, references 4.

The relative total energies calculated in this work of all Nb_3Pb structures listed in the Open Quantum Materials database (OQMD) together with Cmcm-Nb_3Pb can be found in Table S1. The total energy of the Cmcm-Nb_3Pb is set to 0 eV/atom compared to other structures. It can be found that the relative total energy of A15-Nb_3Pb is about 7.6 meV/atom above that of Cmcm-Nb_3Pb, which can imply that Cmcm-Nb_3Pb is more stable than other possible Nb_3Pb compounds at atmospheric pressure

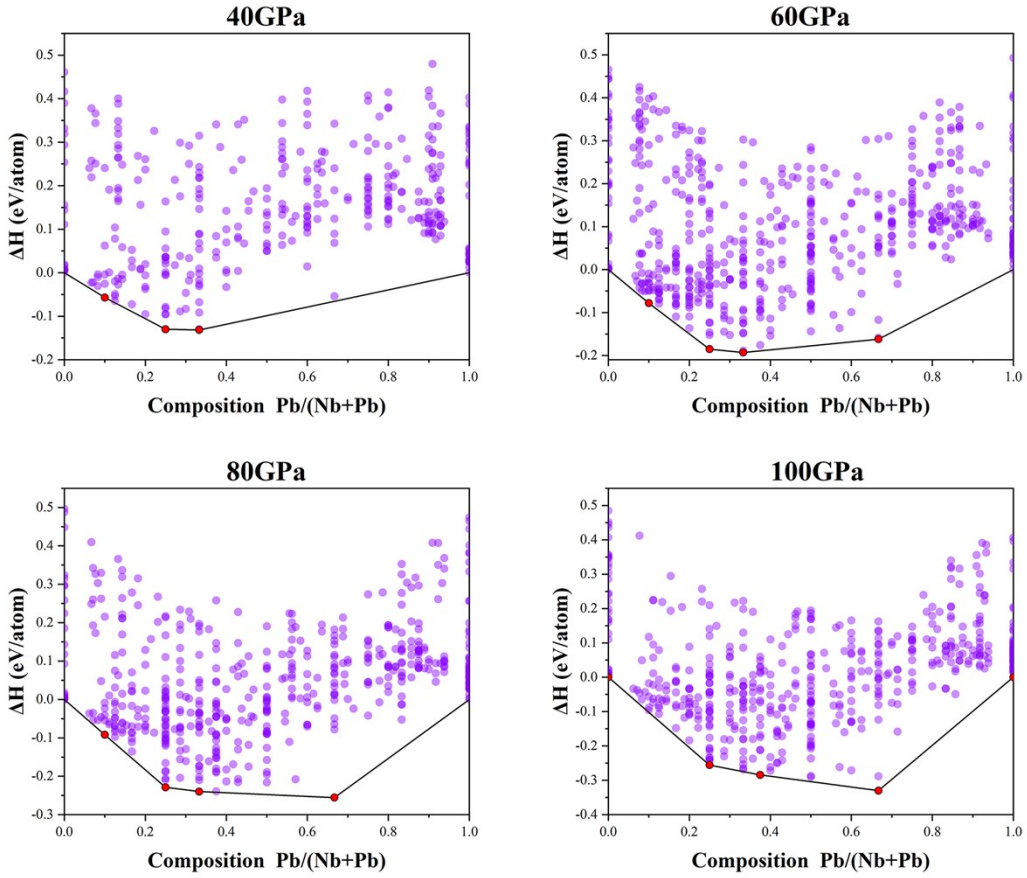

Fig. S1 The illustration of the global structure search of the Nb-Pb system at pressures.

Table S2 The optimized crystal parameters of the Nb-Pb intermetallics (at 0 GPa).

Compounds	Lattice parameters (Å, °)	Atoms	**x**	**y**	**z**
I4/mmm-$NbPb_2$	a=b=c=5.02476	Nb (2b)	1/2	1/2	0
	α=β=140.9438	Pb (8h)	0.17491	0.17491	0
	γ=56.4231	Pb (8h)	0.82509	0.82509	1
Pmm2-Nb_5Pb_3	a=3.19062	Nb (1d)	1/2	1/2	0.73358
	b=4.23137	Nb (1b)	0	1/2	0.27888
	c=8.54208	Nb (1a)	0	0	0.50710
	α=β=γ=90.0000	Nb (1b)	0	1/2	0.22745
		Nb (1c)	1/2	0	0.26940
		Pb (1c)	1/2	0	0.75581
		Pb (1a)	0	0	0.02315
		Pb (1d)	1/2	1/2	0.47907
I4/mmm-Nb_2Pb	a=b=c=5.02476	Nb (8h)	0.17491	0.17491	0
	α=β=140.9438	Nb (8h)	0.82509	0.82509	1
	γ=56.4231	Pb (2b)	1/2	1/2	0
Cmcm-Nb_3Pb	a=b=5.71134	Nb (8g)	0.36483	0.63517	3/4
	c=4.70318	Nb (8g)	0.63517	0.36483	1/4
	α=γ=90.0000	Nb (8g)	0.84323	0.64219	3/4
	β=114.0557	Nb (8g)	0.64219	0.84323	1/4
		Nb (8g)	0.35781	0.15677	3/4
		Nb (8g)	0.15677	0.35781	1/4
		Pb (8g)	0.84954	0.15046	3/4
		Pb (8g)	0.15046	0.84954	1/4
P4/m-Nb_9Pb	a=b=7.14754	Nb (1a)	0	0	0
	c=3.29985	Nb (4k)	0.11088	0.70148	1/2
	α=β=γ=90.0000	Nb (4j)	0.18234	0.39329	0
		Nb (4k)	0.29852	0.11088	1/2
		Nb (4j)	0.39329	0.81766	0
		Nb (4j)	0.60671	0.18234	0
		Nb (4k)	0.70148	0.88912	1/2
		Nb (4j)	0.81766	0.60671	0
		Nb (4k)	0.88912	0.29852	1/2
		Pb (1d)	1/2	1/2	1/2

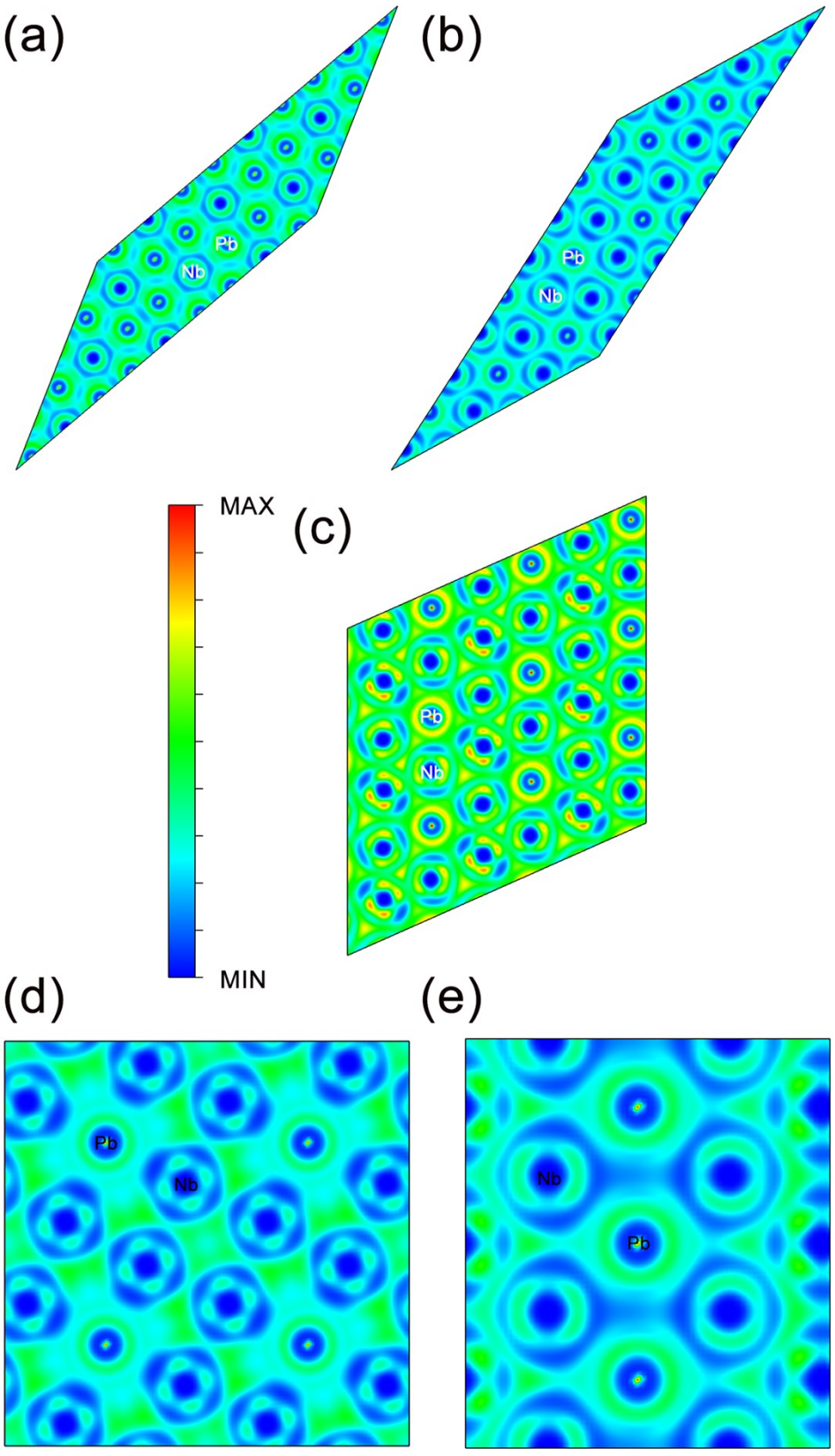

Fig. S2 The Electron Localization Function (ELF) of $NbPb_2$ (a), Nb_2Pb (b), Nb_3Pb (c), Nb_9Pb (d) and Nb_5Pb_3 (e).

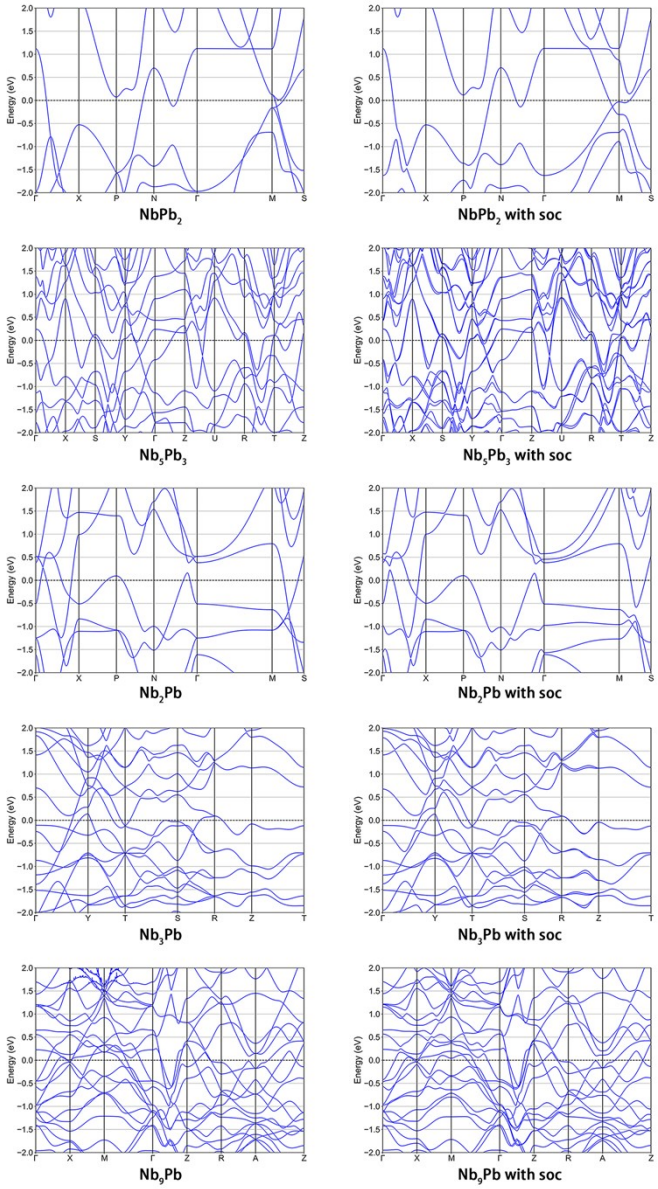

Fig. S3 The energy band structures of Nb-Pb intermetallics with soc and without soc.