Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for the paper entitled "Unexpected superhard phases of Niobium Triborides: first-principles calculations "

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Supplementary information

The reliabilities of the pseudopotentials at high pressures are crosschecked with the full-potential linearized augmented plane-wave (LAPW) method as implemented in the WIEN2k code [1]. By using the two different methods, we calculate total energies of NbB_3 in the $P6_3/mmm$ structure with varying pressures, and then fit the obtained energy-volume data into the Birch-Murnaghan equation of states. Figure S1 shows the resulted fitted equation of states. We can see the results derived from two methods are very small, which clearly indicates the suitability of the PAW pseudopotentials for describing the energetics of NbB_3 at pressures.

Supplementary Figure

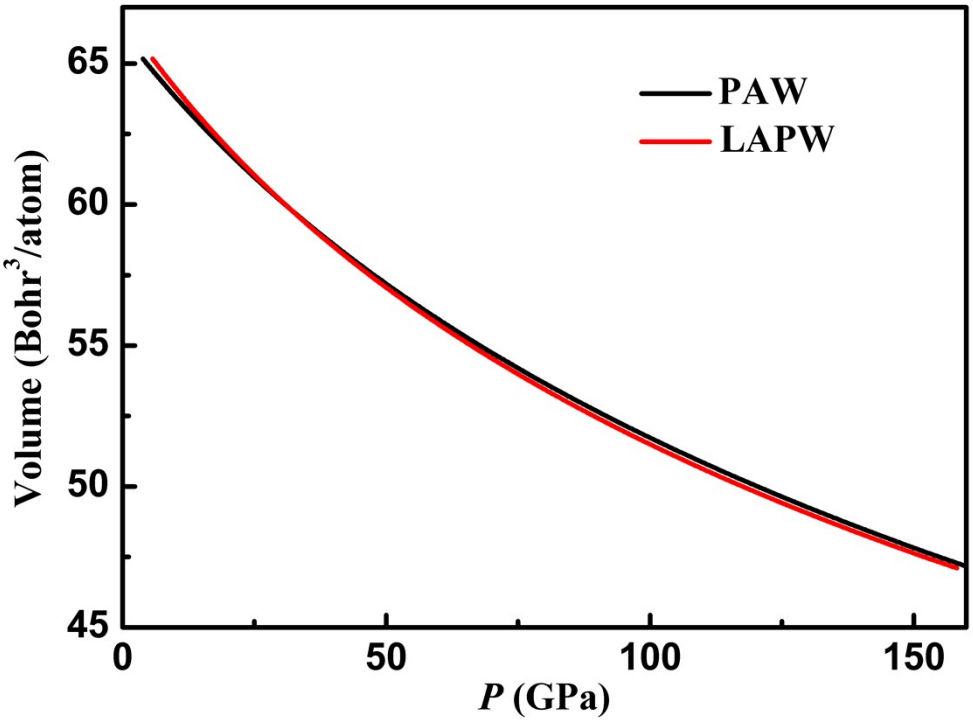

Figure S1. Comparison of the fitted Birch-Murnaghan equation of states for $P6_3/mmm$ phase of NbB_3 by using the calculated results from the PAW pseudopotentials and the full-potential LAPW methods.

Supplementary Table

Table S1 The lattice parameters and atomic positions of all the phases of NbB_3 (the data in the bracket using by LDA method, other calculated by GGA method)

	Lattice parameters (Å)		Atomic coordinates		
*C*2/*c*	*a*=5.325 (5.267)	B (8*f*)	0.3328	0.7076	0.2499
	b=3.064 (3.031)	B (8*f*)	0.8160	0.2928	0.9499
	c=17.831 (17.596)	B (8*f*)	0.0108	0.1924	0.0499
	α=*γ*=90º	Nb (8*f*)	0.5799	0.2073	0.3482
	β=104.5º (105. 9)				
*P*6$_3$/*mmm*	*a*=*b*=5.243 (5.192)	B (6*f*)	0	0.6716	0
	c=3.246 (3.193)	Nb (2*d*)	0.3333	0.6667	0.5
*C*2/*m*	*a*=8.110 (7.959)	B (4*i*)	0.7881	0	0.4756
	b=3.064 (3.005)	B (4*i*)	0.2524	0	0.7040
	c=11.762 (11.561)	B (4*i*)	0.8062	0	0.1289
	α=*γ*=90º	Nb (4*i*)	0.8597	0	0.1683
	β=149.8º (150.1 º)				
*Pmm*2	*a*=3.101 (3.064)	B (4*i*)	0	0	0.2059
	b=3.141 (3.105)	B (4*i*)	0.5	0.5	0.7025
	c=7.246 (7.161)	B (4*i*)	0.5	0.5	0.9484
	α=*γ*=90º	B (4*i*)	0	0.5	0.3179
	β =149.8º (150.1º)	B (4*i*)	0	0.5	0.0729
		B (4*i*)	0	0.5	0.5764
		Nb (1*a*)	0	0	0.8320
		Nb (1*c*)	0.5	0	0.4625
I-4*m*2	*a*=*b*=3.119 (3.082)	B (4*e*)	0	0	0.6265
	c=7.195 (7.105)	B (2*c*)	0	0.5	0.25
		Nb (2*a*)	0	0	0

Reference

[1] P. Blaha, K. Schwarz, P. Sorantin and S.B. Trickey, Comput. Phys. Commun., 1990, **59**, 399.