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Supplementary Information for "New phases in the Ba-Si phase diagram under high pressure by ab initio structural search"

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Table S1 Calculated structural parameters of our predicted stable structures for Ba-Si compounds at their corresponding pressures

Space group Pressure	Lattice parameters	Atomic coordinates (fractional)
Imma-BaSi	a=3.67280 Å	Ba(4e) 0.50000 0.25000 0.39804
20 GPa	b=5.08260 Å	Si(4e) 0.50000 -0.25000 0.17580
	c=9.43680 Å	
	$\alpha=\beta=\gamma=90^\circ$	
$Fd\bar{3}m$-$BaSi_2$	a=7.18670 Å	Ba(8a) 0.25000 0.25000 0.25000
50 GPa	b=7.18670 Å	Si(16d) 0.62500 0.12500 0.12500
	c=7.18670 Å	
	$\alpha=\beta=\gamma=90^\circ$	
$I4/mmm$-$BaSi_3$	a=6.84750 Å	Ba1(4e) 0.50000 0.50000 0.31654
20 GPa	b=6.84750 Å	Ba5(4d) 0.00000 0.50000 0.25000
	c=12.17490 Å	Si1(16m) 0.68117 0.31883 0.09624
	$\alpha=\beta=\gamma=90^\circ$	Si17(8i) 0.66915 0.00000 0.00000
$Cmmm$-$BaSi_5$	a=4.2121 Å	Ba1(2c) 0.00000 0.50000 0.50000
20 GPa	b=7.2510 Å	Si1(8n) -0.00000 0.83323 0.81577
	c=6.3456 Å	Si9(2b) 0.00000 0.50000 -0.00000
	$\alpha=\beta=\gamma=90^\circ$	

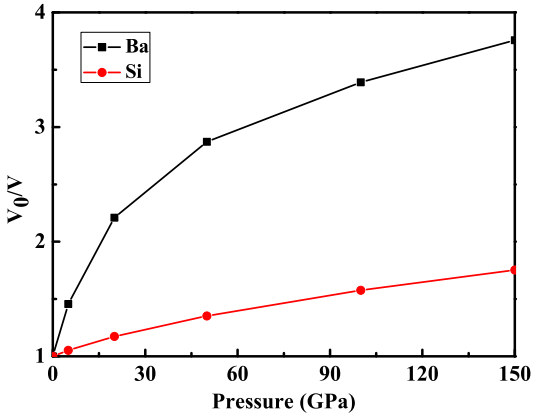

Fig. S1 Compressibility, V0/V, for Ba and Si.

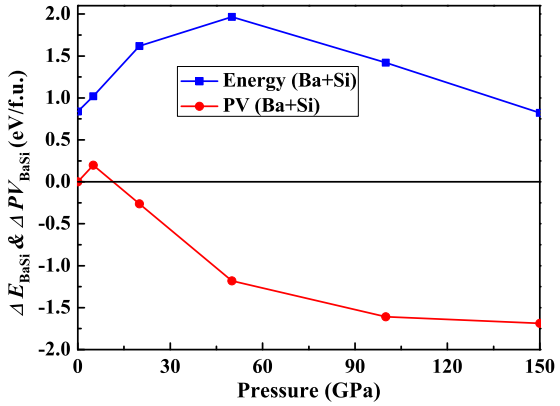

Fig. S2 Ground-state energy and PV components of the enthalpy of the elements relative to BaSi.

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