Supporting Information

Prediction of Metastable Phase of the Sc-N System in the N-rich Region under High Pressure

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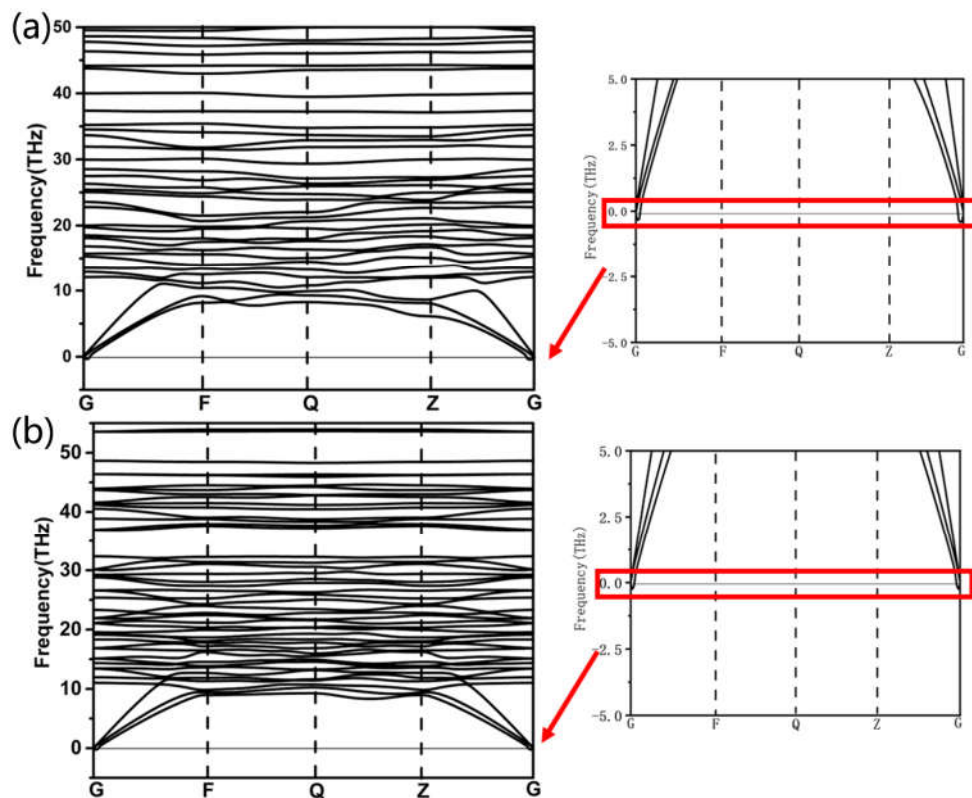* Email: liusj0228@163.com
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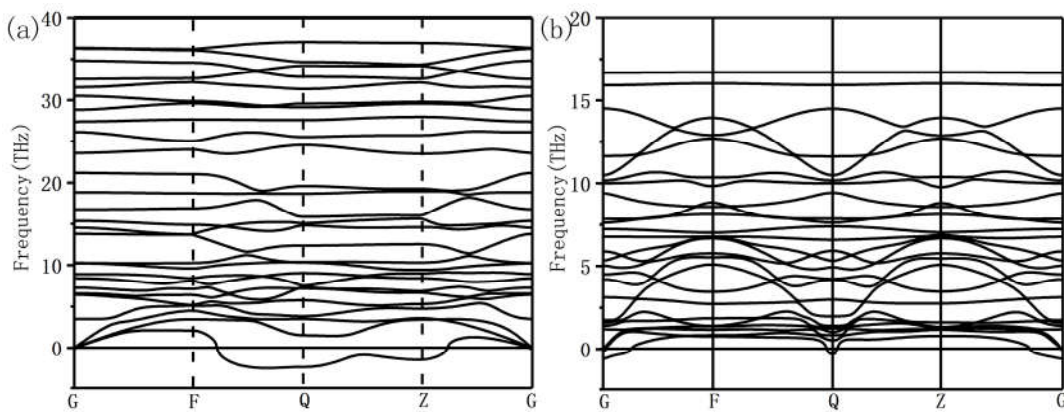**Fig.S1.** The phonon dispersion curves of ScN_{10} (a) and ScN_{14} (b) at 200 GPa.

Fig.S2. The phonon dispersion curves of $P\bar{1}$-ScN_8 (a) and $P1$-ScN_9 (b) at 0 GPa.
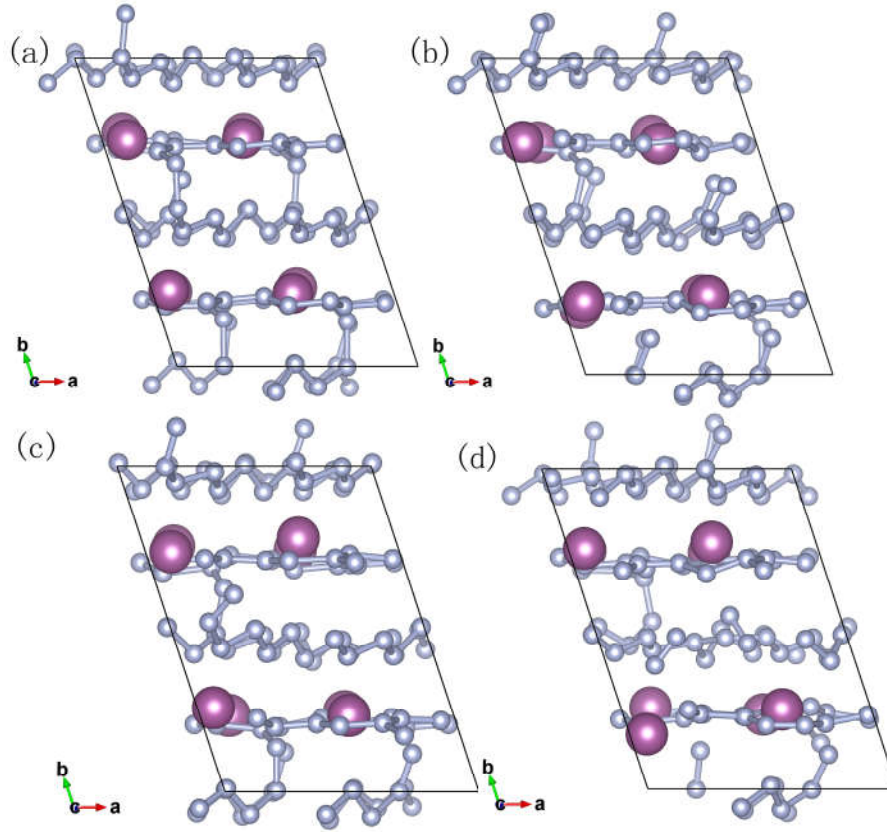
Fig.S3. Images of P1-ScN$_{11}$ after the FPMD simulation: 300 K (a), 600 K (b) and 800 K at 3 ps (c), 10 ps (d) at 0 GPa.

Table S1. The lattice constants and position coordinate of the Sc-N system.

Structure	Pressure (GPa)	Lattice Parameters (Å, °)	Atomic Positions
P$\bar{1}$-ScN$_8$	200	a = 2.6795 b = 4.1986 c = 4.3265 α = 73.02° β = 92.70° γ = 100.62°	Sc$_1$(1g) (0.0000, 0.5000, 0.5000) N$_1$(2i) (0.1254, 0.0598, 0.8580) N$_2$(2i) (0.5187, 0.6863, 0.1270) N$_3$(2i) (0.5534, -0.1450, 0.5841) N$_4$(2i) (0.2727, 0.7686, 0.8496)

P1-ScN$_9$	200	a = 3.4118 b = 4.2794 c = 4.2924 α = 116.05° β = 106.33° γ = 98.79°	Sc$_1$(1a) (0.2809, 0.0731, 0.6178) N$_1$(1a) (0.0469, 0.4712, 0.2403) N$_2$(1a) (0.8898, 0.1535, 0.9351) N$_3$(1a) (0.6447, 0.8168, 0.3480) N$_4$(1a) (0.5555, 0.2933, 0.3834) N$_5$(1a) (0.9588, 0.3948, 0.5089) N$_6$(1a) (0.9503, 0.8857, 0.0207) N$_7$(1a) (0.5537, 0.6591, 0.9843) N$_8$(1a) (0.1810, 0.7211, 0.8306) N$_9$(1a) (0.1810, 0.7211, 0.8306)
P1-ScN$_{11}$	200	a = 3.4893 b = 4.3073 c = 4.5362 α = 102.29° β = 99.94° γ = 107.61°	Sc$_1$(1a) (0.1682, 0.5279, 0.5496) N$_1$(1a) (0.4410, 0.9184, 0.9413) N$_2$(1a) (0.4336, 0.4504, 0.1399) N$_3$(1a) (0.7872, 0.8398, 0.6362) N$_4$(1a) (0.5052, 0.3746, 0.8598) N$_5$(1a) (0.0934, 0.8342, 0.2917) N$_6$(1a) (0.0264, 0.3127, 0.0735) N$_7$(1a) (0.5661, 0.3247, 0.3601) N$_8$(1a) (-0.0059, 0.0241, 0.4906) N$_9$(1a) (0.8230, 0.9725, 0.9272) N$_{10}$(1a) (0.8737, 0.4395, 0.8642) N$_{11}$(1a) (0.4295, 0.9932, 0.2276)