Supporting Information

Pressure tuned incommensurability and guest structure transition in compressed scandium from machine learning atomic simulation

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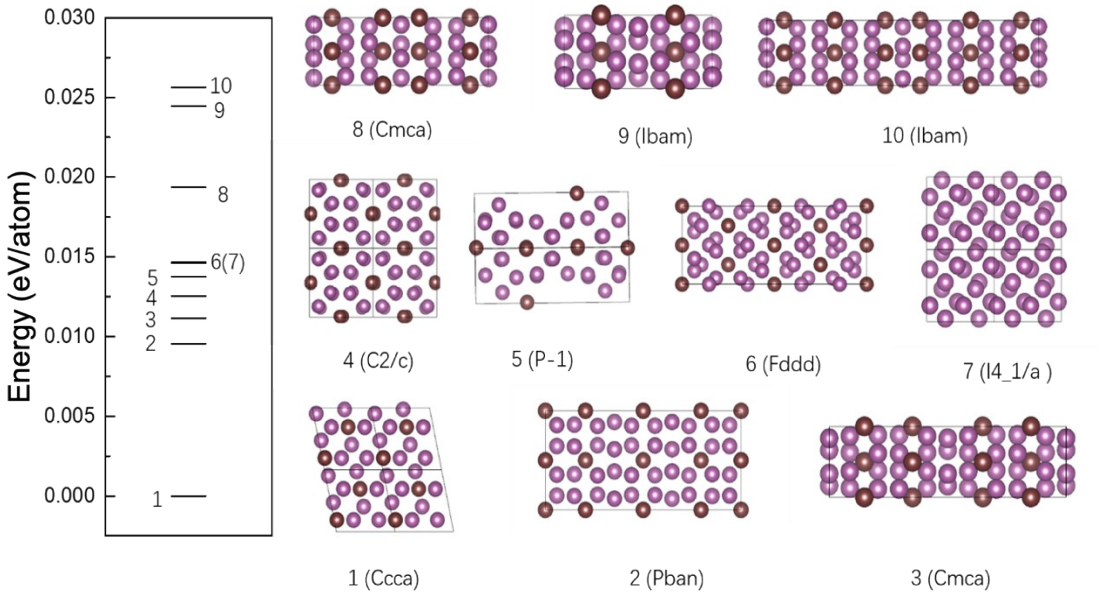

Fig. S1. Configurational energy spectra at 90 GPa from DFT calculation. The **Structure 1-3**, and **6-10** are the ordinary structures, while **Structure 4 is** HG structure with bcm guest configuration (γ=1.333), **and Structure 5** is HG structure with fcm guest configuration (γ=1.343), both the host framework and guest structure are distorted.

Table S1 10 minimum structure and energy calculation (relative to *Ccca structure*) comparison between DFT and NN at 90 GPa.

Number	Symttery	DFT/eV	NN/eV	E_{diff}/meV	Space
1	*Ccca*	2.971836	2.975333	3.4965	68
2	*Pban*	2.981398	2.982279	0.880437	50
3	*Cmca*	2.982987	2.978436	4.5515	64
4	*C*2/*c*	2.984378	2.989537	5.158781	15
5	*P*-1	2.985592	2.993147	7.555146	2
6	*Fddd*	2.986451	2.991146	4.695438	70
7	$I4_1/a$	2.986513	2.99255	6.036813	88
8	*Cmca*	2.991195	2.991704	0.509875	64
9	*Ibam*	2.996282	2.987591	8.691143	72
10	*Ibam*	2.99748	2.987179	10.30085	72

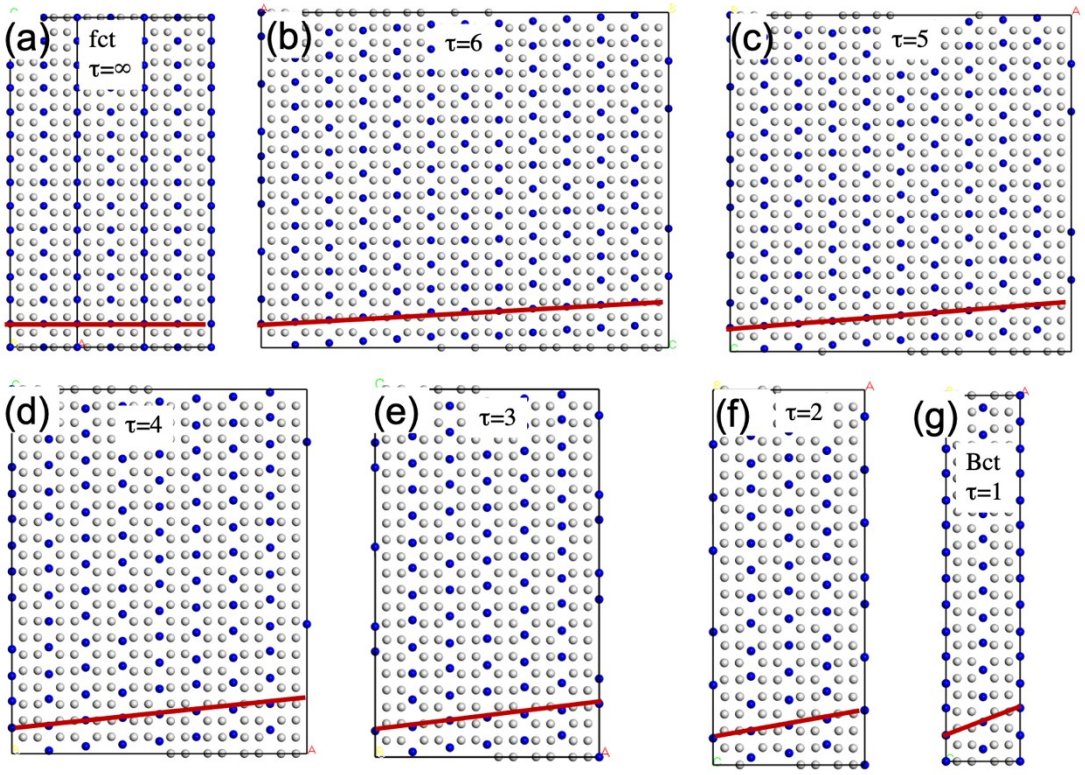

Fig. S2. The same incommensurate ratio (γ=14/11) H-G structure with different guest configuration. (a) H-G structure with fct guest configuration, (b-f) H-G structure with τ=2, 3, 4, 5, and 6 in fcm and bcm guest configuration. (g) the H-G structure with bct guest configuration. The red lines (in ab plane) guard how the original fct guest transit to bct guest.

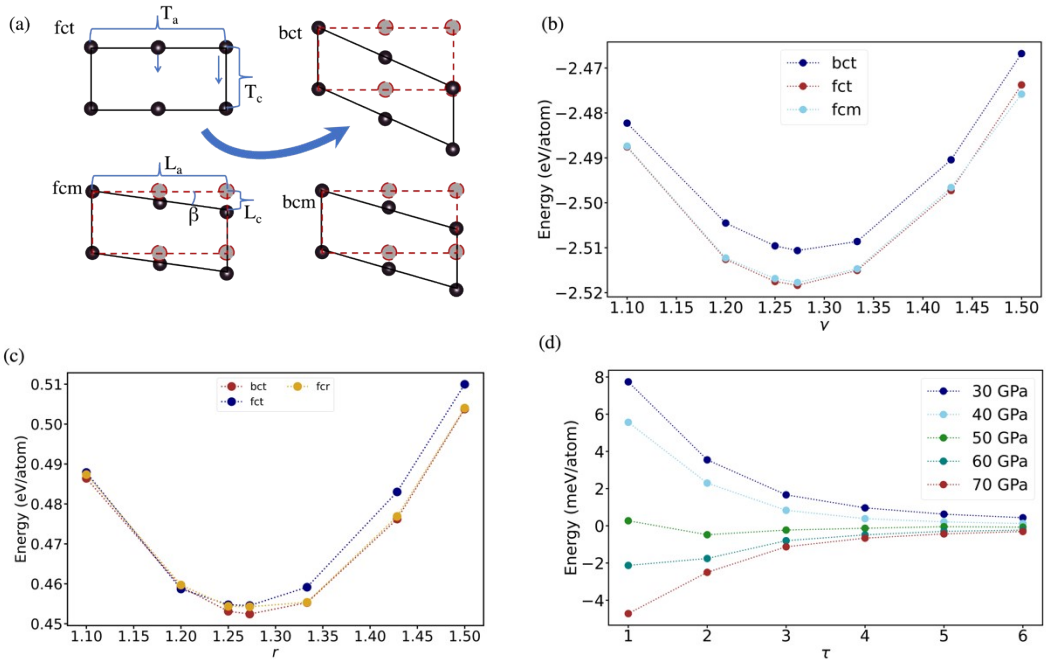

Fig. S3. (**a**) The scheme of *fct* to *bct* via *fcm* and *bcm*. The energies vs γ at 30 GPa (**b**), and 60 GPa (**c**), the fcm is τ=5 with γ=14/11. (**d**) The relative energies of *fct* (γ=14/11) with τ from 2 to 6, *fct* and *bct* at 30, 40, 50, 60, 70 GPa.

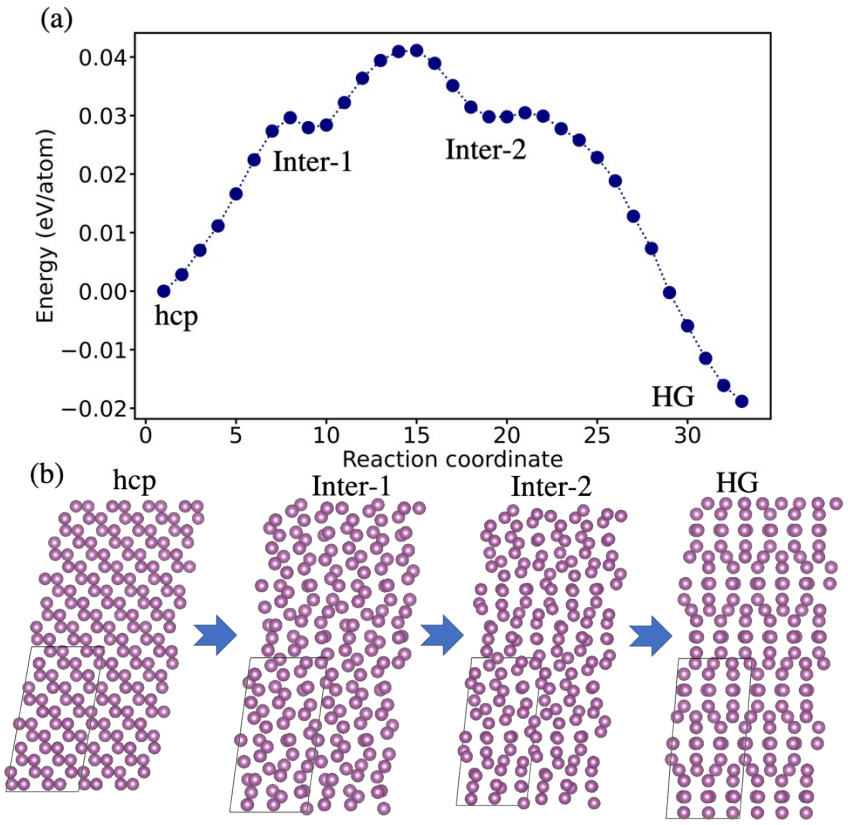

Fig. S4. (a) The energy profile of 48-atom pathway which calculated by neural network potential; **(b)** the key structural snaps of the phase transition path. The energy barrier is 0.041 eV/atom. Inter-1 and Inter-2 are two shallow intermediate structures along the hcp to HG structure phase transition.

Structure information of transition pathway

32-atom phase transition pathway

Hcp structure

PBC 7.29163364 7.29176015 10.47955126 89.99970291 90.00009430 91.66525594

Sc 5.361422103 5.005009328 2.608710534 CORE 1 Sc Sc 0.0000 1
Sc -0.125296971 6.863316860 7.848618052 CORE 2 Sc Sc 0.0000 2
Sc 1.821537702 1.360679640 2.608782050 CORE 3 Sc Sc 0.0000 3
Sc 1.422896620 4.703796683 8.900625468 CORE 4 Sc Sc 0.0000 4
Sc 1.820732233 1.359899758 7.848606884 CORE 5 Sc Sc 0.0000 5
Sc 6.088470433 7.258396435 10.468545689 CORE 6 Sc Sc 0.0000 6
Sc 5.360626075 5.004223436 7.848678495 CORE 7 Sc Sc 0.0000 7
Sc 0.271341625 3.518269117 3.660834052 CORE 8 Sc Sc 0.0000 8
Sc 5.174617589 1.059356909 6.796839467 CORE 9 Sc Sc 0.0000 9
Sc 0.271377739 3.518374257 6.796762118 CORE 10 Sc Sc 0.0000 10
Sc 5.237025526 3.388175663 5.228572174 CORE 11 Sc Sc 0.0000 11
Sc 3.811195046 7.162620019 1.556830335 CORE 12 Sc Sc 0.0000 12
Sc 1.393226730 2.424613992 10.468528158 CORE 13 Sc Sc 0.0000 13
Sc -0.124483567 6.864137958 2.608699985 CORE 14 Sc Sc 0.0000 14
Sc 5.174573212 1.059318222 3.660523330 CORE 15 Sc Sc 0.0000 15
Sc 2.548669427 3.614099084 5.228517821 CORE 16 Sc Sc 0.0000 16
Sc 2.617120825 5.933221716 6.811002908 CORE 17 Sc Sc 0.0000 17
Sc 6.368942505 2.288899147 1.571210852 CORE 18 Sc Sc 0.0000 18
Sc 1.485221502 7.032562669 10.468541974 CORE 19 Sc Sc 0.0000 19
Sc 3.748615421 4.833982309 10.468526622 CORE 20 Sc Sc 0.0000 20
Sc 3.626466643 3.218979405 7.848574077 CORE 21 Sc Sc 0.0000 21
Sc 3.811183509 7.162618832 8.900726319 CORE 22 Sc Sc 0.0000 22
Sc 6.368870587 2.288879798 8.886424965 CORE 23 Sc Sc 0.0000 23
Sc 3.627309761 3.219778870 2.608747945 CORE 24 Sc Sc 0.0000 24
Sc 4.933084477 6.068852529 5.228653285 CORE 25 Sc Sc 0.0000 25
Sc 0.208734652 1.189640799 5.228554548 CORE 26 Sc Sc 0.0000 26
Sc 4.052477701 2.153317639 10.468533922 CORE 27 Sc Sc 0.0000 27
Sc 2.617204569 5.933283201 3.646441393 CORE 28 Sc Sc 0.0000 28
Sc 2.897245626 0.963548084 5.228658307 CORE 29 Sc Sc 0.0000 29
Sc 6.437173782 4.607937866 10.468535430 CORE 30 Sc Sc 0.0000 30
Sc 0.300785874 5.797694031 5.228503014 CORE 31 Sc Sc 0.0000 31
Sc 1.422852725 4.703665273 1.557150982 CORE 32 Sc Sc 0.0000 32

end

end

H-g structure

PBC 6.93961351 7.53187214 11.29007716 104.59126900 93.81034549 84.29825723

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Sc      5.906333349    4.291379156    1.581115315 CORE    1 Sc Sc   0.0000    1
Sc     -0.126579838    5.133132698    9.311581484 CORE    2 Sc Sc   0.0000    2
Sc      2.062218130    1.132858014    2.945902583 CORE    3 Sc Sc   0.0000    3
Sc      2.061197879    3.488445681    8.403742664 CORE    4 Sc Sc   0.0000    4
Sc      1.047467919   -1.370942381    7.264693966 CORE    5 Sc Sc   0.0000    5
Sc      4.890728121    4.143242039   11.358373049 CORE    6 Sc Sc   0.0000    6
Sc      4.891205759    2.965088170    8.629368780 CORE    7 Sc Sc   0.0000    7
Sc     -0.125547122    2.777562933    3.853740925 CORE    8 Sc Sc   0.0000    8
Sc      5.157165666   -0.847693160    7.039089194 CORE    9 Sc Sc   0.0000    9
Sc      0.139413949    1.320440464    7.721475985 CORE   10 Sc Sc   0.0000   10
Sc      4.891646407    1.787660056    5.900482969 CORE   11 Sc Sc   0.0000   11
Sc      3.718598147    5.936026760    2.489060606 CORE   12 Sc Sc   0.0000   12
Sc      1.046967961   -0.193338991    9.993547394 CORE   13 Sc Sc   0.0000   13
Sc      0.888606395    6.459512595    2.263602166 CORE   14 Sc Sc   0.0000   14
Sc      4.892249875    0.609517920    3.171527584 CORE   15 Sc Sc   0.0000   15
Sc      2.061606820    2.310735867    5.674878512 CORE   16 Sc Sc   0.0000   16
Sc      3.983523997    4.478864561    6.356904117 CORE   17 Sc Sc   0.0000   17
Sc      6.814435040    1.600208615    1.124676461 CORE   18 Sc Sc   0.0000   18
Sc      2.060748421    4.666280052   11.132776079 CORE   19 Sc Sc   0.0000   19
Sc      2.968911183    1.974907725   10.675775225 CORE   20 Sc Sc   0.0000   20
Sc      2.969253371    0.797090910    7.946910931 CORE   21 Sc Sc   0.0000   21
Sc      3.983047886    5.656322411    9.085808791 CORE   22 Sc Sc   0.0000   22
Sc      5.156630035    0.329741787    9.767906247 CORE   23 Sc Sc   0.0000   23
Sc      3.984062452    3.300776433    3.627964860 CORE   24 Sc Sc   0.0000   24
Sc      5.905987774    5.468748747    4.310116427 CORE   25 Sc Sc   0.0000   25
Sc      0.139867073    0.142382306    4.992635940 CORE   26 Sc Sc   0.0000   26
Sc      3.234329173   -0.660228269   11.814795567 CORE   27 Sc Sc   0.0000   27
Sc      1.796261756    4.945693174    4.535748092 CORE   28 Sc Sc   0.0000   28
Sc      2.969771209   -0.380610047    5.217949055 CORE   29 Sc Sc   0.0000   29
Sc      7.078460701    2.498040567   10.450437466 CORE   30 Sc Sc   0.0000   30
Sc     -0.126017111    3.955691105    6.582691745 CORE   31 Sc Sc   0.0000   31
Sc      1.796657035    3.768070228    1.806740342 CORE   32 Sc Sc   0.0000   32
end
end


42-atom phase transition pathway
Hcp structure
PBC   7.23849183   11.84488570    9.82627607   69.15778951  101.40597487   77.17319790
Sc      6.713550014    5.828863624    4.547355210 CORE    1 Sc Sc   0.0000    1
Sc      5.564274372   11.145488282    3.450548665 CORE    2 Sc Sc   0.0000    2
Sc      6.873178175    7.525592148    1.948418805 CORE    3 Sc Sc   0.0000    3
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Sc     5.566926900  13.470564906   4.921656923 CORE   4 Sc Sc   0.0000   4
Sc     2.792544819   4.540885617   8.037659026 CORE   5 Sc Sc   0.0000   5
Sc     3.212719455   9.130723810   5.430550469 CORE   6 Sc Sc   0.0000   6
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Sc     7.847890044   9.616017797   4.053601642 CORE   8 Sc Sc   0.0000   8
Sc    -0.789933745   2.941051191   4.537695895 CORE   9 Sc Sc   0.0000   9
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Sc     2.916300445  10.962080869   3.212404172 CORE  12 Sc Sc   0.0000  12
Sc     1.796260176   4.334058238   5.093815471 CORE  13 Sc Sc   0.0000  13
Sc     4.409162974   9.270967371   8.165338629 CORE  14 Sc Sc   0.0000  14
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Sc     7.841561510  12.047343463   5.388317097 CORE  23 Sc Sc   0.0000  23
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Sc     2.853575007   1.363725608   1.070848166 CORE  25 Sc Sc   0.0000  25
Sc     5.604885892  10.602199772   6.171256137 CORE  26 Sc Sc   0.0000  26
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Sc     5.574589911  13.026688794   7.662303737 CORE  34 Sc Sc   0.0000  34
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Sc     0.999509691  13.115469048   7.789283773 CORE  36 Sc Sc   0.0000  36
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Sc     2.921091845   8.609876073   1.799591048 CORE  38 Sc Sc   0.0000  38
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H-g structure

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227 end
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