

*Structural systematic
in the
phase-diagrams
of the
elements*

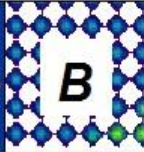





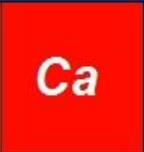











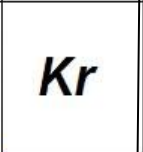













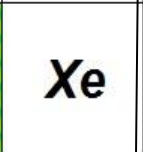







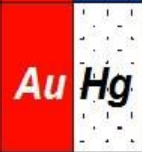





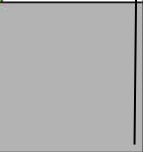

A simple guide to the world of high pressure
AIRAPT lecture 2023

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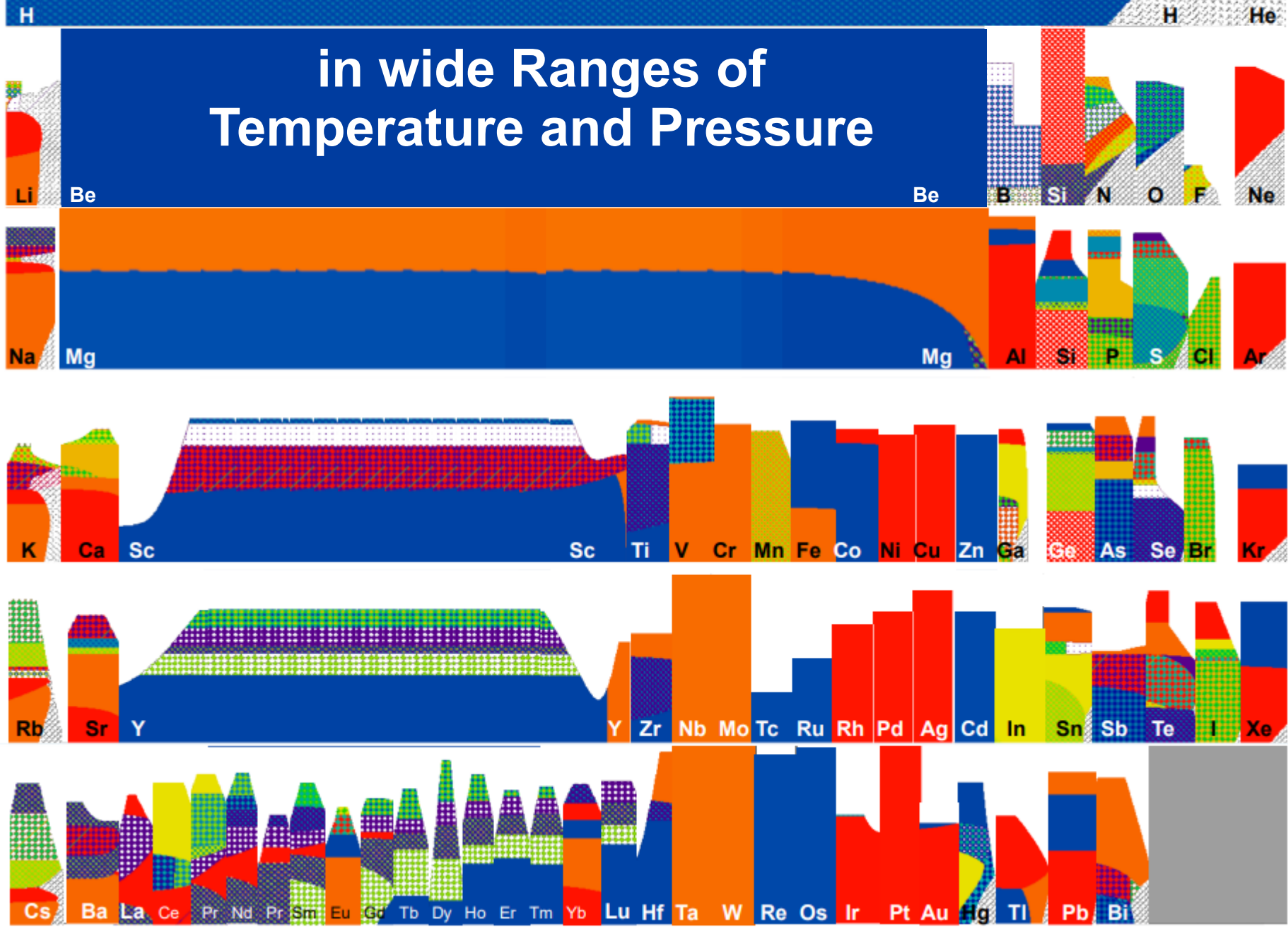
Crystal Structures of the Elements at ambient Pressure

H															H	He		
Li	Be											Be	 B	 C	N	O	F	Ne
Na	Mg											Mg	 Al	 Si	 P	 S	Cl	Ar
K	 Ca	 Sc	 Ti	 V	 Cr	 Mn	 Fe	 Co	 Ni	 Cu	 Zn	 Ga	 Ge	 As	Se	Br	Kr	
Rb	 Sr	 Y	 Zr	 Nb	 Mo	 Tc	 Ru	 Rh	 Pd	 Ag	 Cd	 In	 Sn	 Sb	Te	J	Xe	
Cs	 Ba	 La....Lu	 Hf	 Ta	 W	 Re	 Os	 Ir	 Pt	 Au	 Hg	 Tl	 Pb	 Bi				

Key for the Crystal Structures

cl2 	hP2 	hR105 	cF4 	cF8 	oC8 
cl58 	hR2 	hR3 	tl2 	tl4 	oF128 

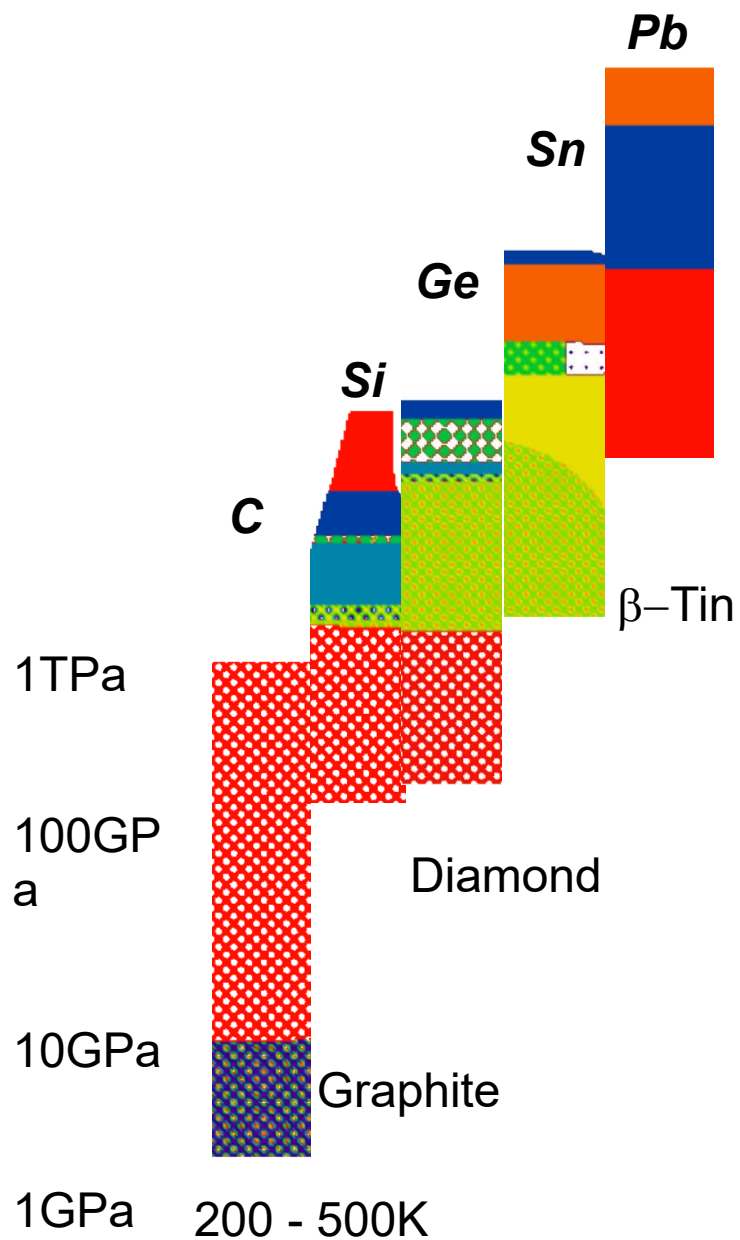
The colorful World of the Elements



in wide Ranges of
Temperature and Pressure

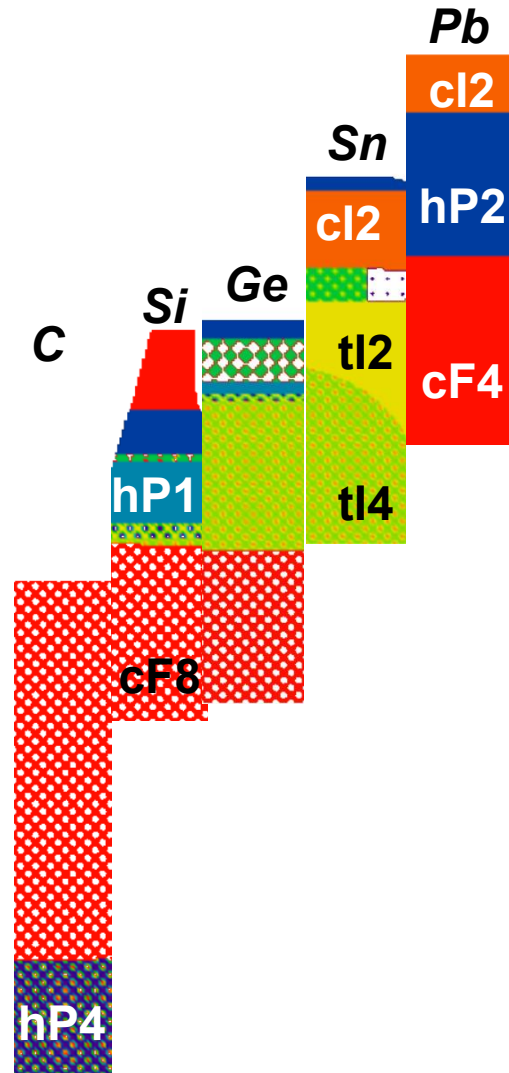
The Carbon Group

Smaller values for the ratio of atomic versus ionic radii result in high pressure structures.
Heavier Elements start with smaller radius ratios.



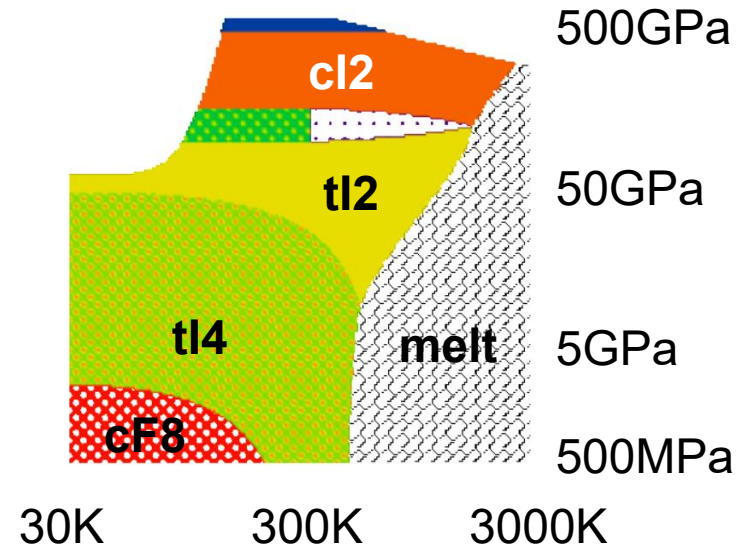
The Carbon Group

Section 1TPa
to
Diagrams 1GPa
200 to 500K



C	hP4	----	cF8	----	>275GPa										
ptr/GPa	3														
Si	cF8	----	tI4	----	oI4	----	hP1	----	oC16	----	hP2	----	cF4	----	>250GPa
ptr/GPa	12	13	16	38	42	80									
Ge	cF8	----	tI4	----	oI4	----	hP1	----	oC16	----	hP2	----	>180GPa		
ptr/GPa	11	75	85	102	160										
Sn	cF8	----	tI4	----	tI2	----	oI2	----	cl2	----	hP2	----	>194GPa		
ptr/GPa	0	9.2	32	70	157										
Pb	cF4	----	hP2	----	cl2	----	>272GPa								
ptr/GPa	13	127													

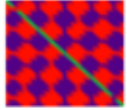
Sn: 30-3000K, 0.5-500GPa



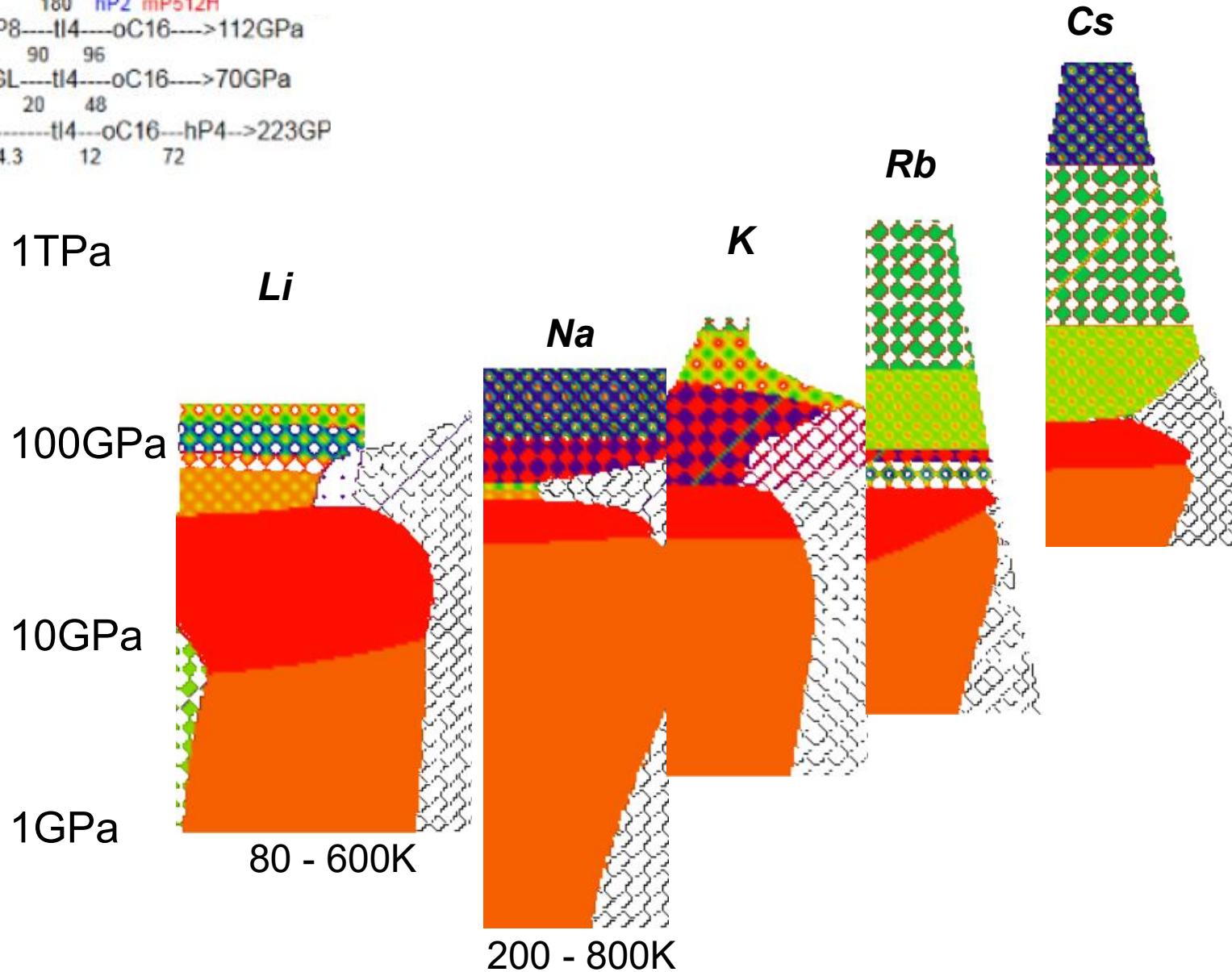
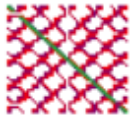
The Alkaline Metals

Li	cl2	cF4	liquid	oC40	oC24	>116GPa
ptr/GPa	7.5	39		75	90	
200K:	hR1	cl16	oC88	oC40	oC24	
Na	cl2	cF4	cl16	oP8***	HGL	hP4->215GPa
ptr/GPa	65	104	115	125	180	hP2 mP512H
K	cl2	cF4	HGL	oP8	tl4	oC16->112GPa
ptr/GPa	11.6	20		54	90	96
Rb	cl2	cF4	oC52	HGL	tl4	oC16->70GPa
ptr/GPa	7	13	17	20	48	
Cs	cl2	cF4	oC84	tl4	oC16	hP4->223GP
ptr/GPa	2.4	4.2		4.3	12	72

Different types of **ordered HGL** host-guest lattices are represented by



disordered HGD host-guest lattices are represented by



The Nitrogen Group

N	gas	hP4	cP16	tP32	hR8	oP16	cl8	>120GPa
ptr/GPa	2.6	4.7	8	18	50	115	cP8 tP4	
P	oC8	hR2	cP1	ML	hP1	cl2	>280GPa	
ptr/GPa	5	10	107	137	258			
As	hR2	cP1	HGL	cl2	>122GPa			
ptr/GPa	25	48	97					
Sb	hR2	HGL	HGL	cl2	>65GPa			
ptr/GPa	8.2	9.0	28					
Bi	hR2	mC4	HGL	cl2	>220GPa			
ptr/GPa	2.5	2.7	7.7	oC16Hf				

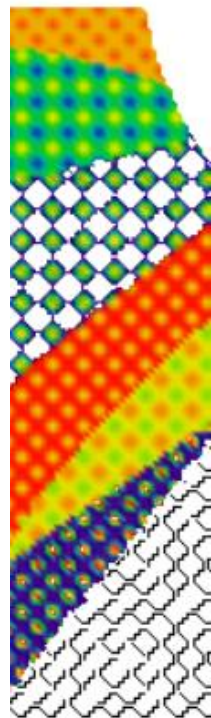
1TPa

100GPa
a

10GPa

1GPa

N



200 - 500K

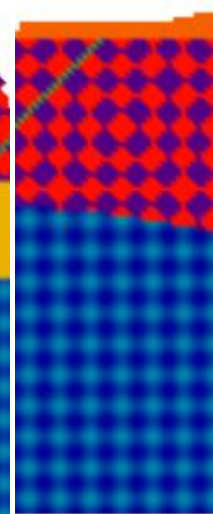


P

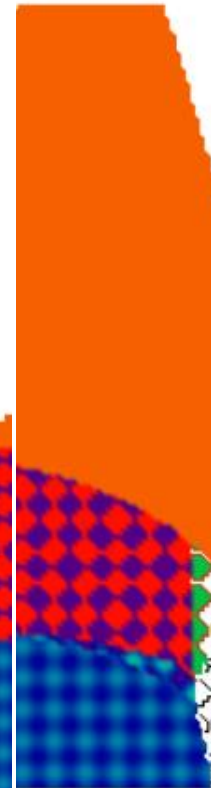
As



Sb



Bi



1TPa

100GPa
a

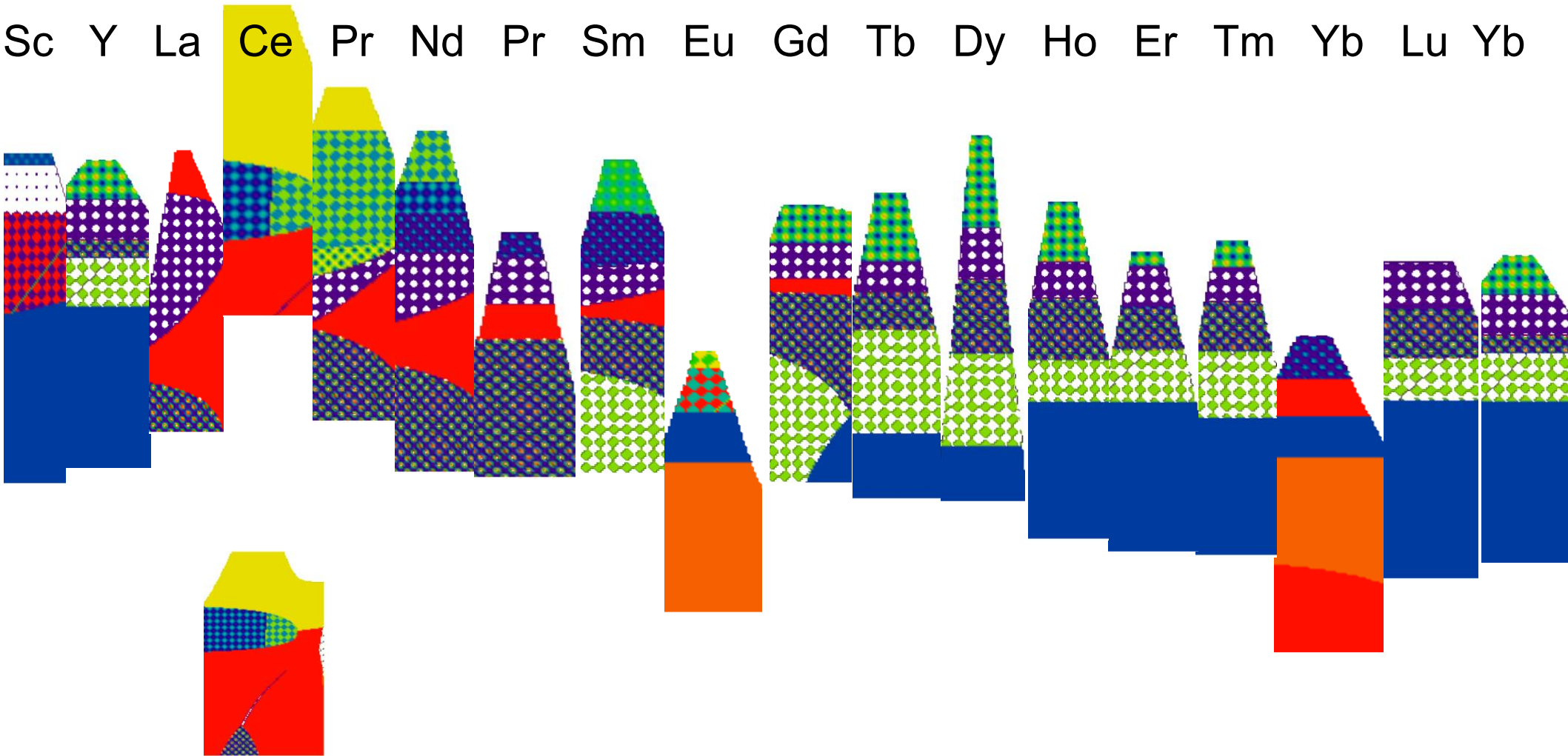
10GPa

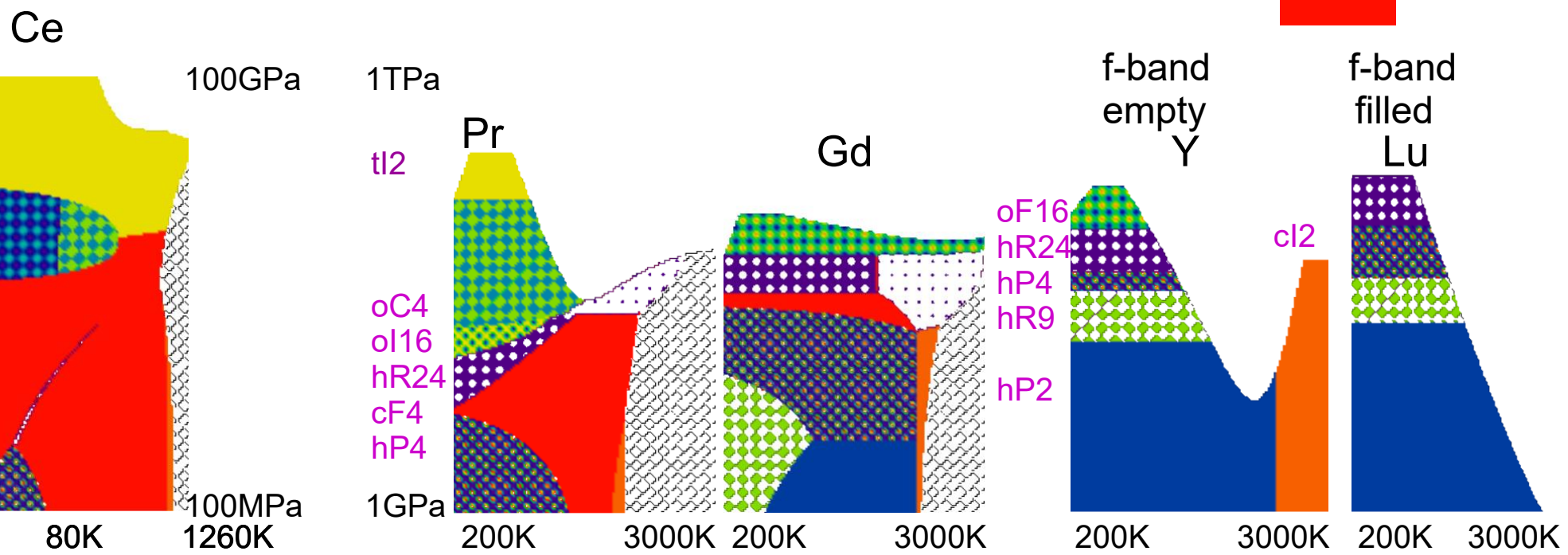
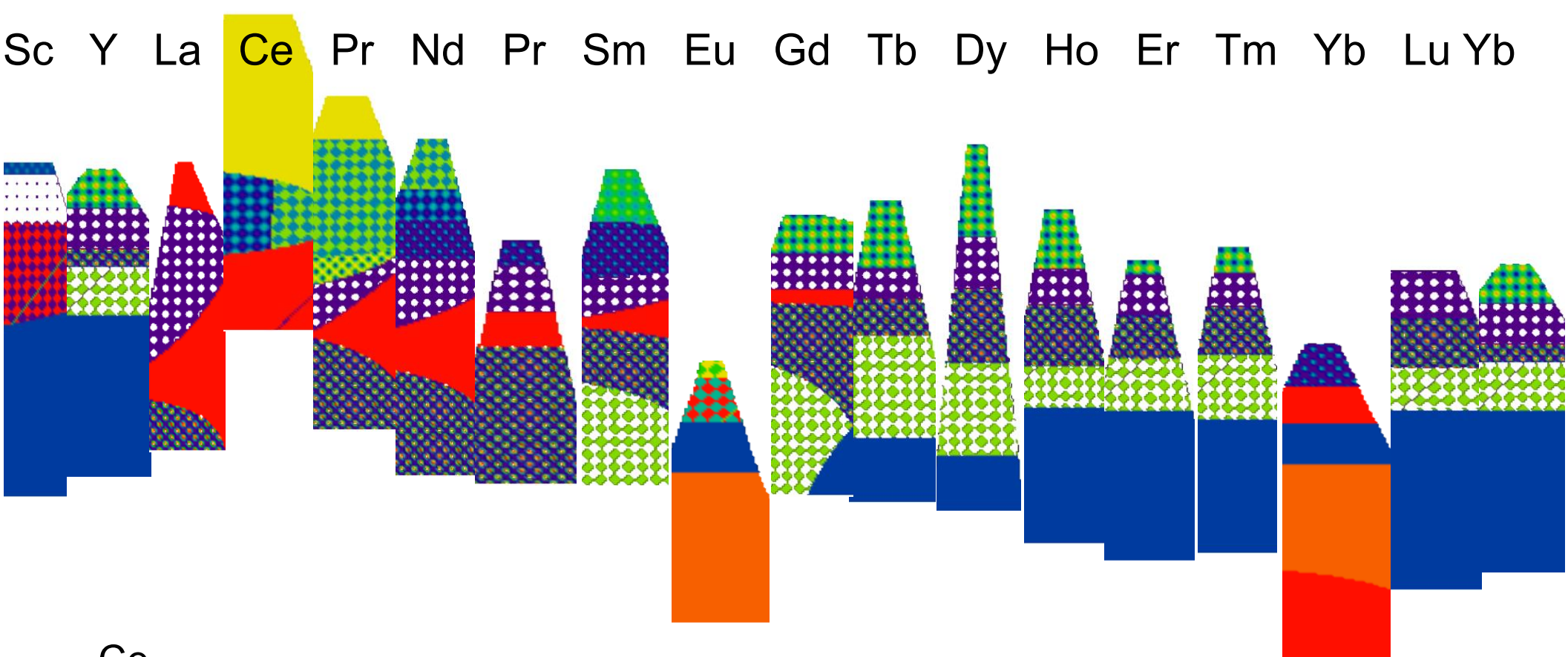
1GPa

La hP4—cF4—hR8—cF4—>70GPa
 ptr/GPa 2 7 58 d2HT
Ce hP4—cF4—cF4—oC4—II2—>208GPa
 ptr/GPa 2 .87 3.9 13 d2HT
Pr hP4—cF4—hR8—???—oC4—>60GPa
 ptr/GPa 4 6.2 10 20 d2HT
Nd hP4—cF4—hR8—hP3—mC4—oC4—>70GPa
 ptr/GPa 5 15 40 75 113 d2HT
Pm hP4—cF4—hR8—hP3—>60GPa
 ptr/GPa 10 18 40
Sm hR3—hP4—cF4—hP3—II2—mC4—>70GPa
 ptr/GPa 5 15 75 105 d2HT
Eu cI2—hP2—MI 12GPa
 ptr/GPa 13 31.5

Gd hP2—hR3—hP4—cF4—hR8—mI2—>235GPa
 ptr/GPa 3.2 7 26 46 61 d2HT
Tb hP2—hR3—hP4—cF4—hR8—>58GPa
 ptr/GPa 3 6 29 32
Dy hP2—hR3—hP4—cF4—hR8—>70GPa
 ptr/GPa 5 9 38 40
Ho hP2—hR3—hP4—hR8—>70GPa
 ptr/GPa 10 25 70
Er hP2—hR3—hP4—hR8—>70GPa
 ptr/GPa 12.4 24 67.4
Tm hP2—hR3—hP4—>42GPa
 ptr/GPa 10 30
Yb hP2—cF4—cI2—hP2—cF4—hP3—>202GPa
 ptr/GPa 0.1 4 30 53 98
Lu hP2—hR3—hP4—cF4—Lu(IV)—>275GPa
 ptr/GPa 20 30 88 272

Sc Y La Ce Pr Nd Pr Sm Eu Gd Tb Dy Ho Er Tm Yb Lu Yb





IA

H gas---hP4H---->200GPa
ptr/GPa 5.3 hP4B hP4D

Li cl2---cF4-- liquid --oC40----oC24-->116GPa [MN06,VD06,OD09,GG11]
ptr/GPa 7.5 39 75 90 hR3
200K: hR1---cl16---oC88-----oC40-----oC24

Na cl2---cF4---cl16--oP8***--HGL--hP4->215GPa [GD05,MN06,VD06,GL08,LG09,ME09,OD09]
ptr/GPa 65 104 115 125 180 hP2 mP512HT oP8*** includes tl50 oC120 aP90

K cl2---cF4---HGL---oP8---tl4---oC16---->112GPa [MN06,VD06,OD09]
ptr/GPa 11.6 20 54 90 96

Rb cl2---cF4---oC52---HGL---tl4---oC16---->70GPa [MN06,VD06,OD09]
ptr/GPa 7 13 17 20 48

Cs cl2---cF4---oC84-----tl4---oC16---hP4-->223GPa [MD03,MN06,VD06,OD09]
ptr/GPa 2.4 4.2 4.3 12 72

IIA

[MN06, VD06, OD09]

Be hP2----->171GPa
ptr/GPa

Mg hP2-----cl2----->58GPa [YK12]
ptr/GPa 50

Ca cF4--cl2--cP1---tP8---oC8---mC6---HGL->216GPa [YN05,VD06,NY07, FN08,MW10,NS10]
ptr/GPa 20 32 113 139 158 210 oC2 tl4 [OM10,SN11,TD12,LD12, FN13,VD14]

Sr cF4 ---cl2---tl4---ml12---HGL---->117GPa [BA05]
ptr/GPa 3.5 27 35 49

Ba cl2-----hP2-----HGL-----hP2----->105GPa
ptr/GPa 5.5 12 45 cF4HT

IIIA

[MN06,VD06]

B hR106-----hR12-----oP28---oC8---->250GPa [BT04,OC09,OS11]
ptr/GPa 3 tP192HT 18 89

Al cF4-----hP2----> 333GPa [AN06]
ptr/GPa 217

Ga oC8---liquid---tl2---oC104---hR6---tl2---cF4--->150GPa [DM04,MN06]
ptr/GPa 0 2.0 2.8 tl2HT 10.5 14 120

In tl2---oF4---->93GPa
ptr/GPa 45

Tl hP2---cF4---->68GPa
ptr/GPa 3.7 cl2HT

IVA

C	hP4----cF8---->275GPa	
ptr/GPa	3	
Si	cF8---tl4----ol4----hP1---oC16----hP2----cF4---->250GPa	
ptr/GPa	12 13 16 38 42 80	
Ge	cF8---tl4----ol4----hP1---oC16----hP2---->180GPa	
ptr/GPa	11 75 85 102 160	
Sn	cF8---tl4----tl2---ol2---cl2----hP2---->194GPa	[SG11,SB13]
ptr/GPa	0 9.2 32 70 157	
Pb	cF4----hP2----cl2---->272GPa	
ptr/GPa	13 127	

VA

N	gas---hP4---cP16---tP32---hR8---oP16---cl8-->120GPa	[EG04,GG07,SL09,MO09]
ptr/GPa	2.6 4.7 8 18 50 115 cP8 tP4	
P	oC8---hR2---cP1---ML---hP1---cl2---->280GPa	[VD06,MA08]
ptr/GPa	5 10 107 137 258	
As	hR2---cP1---HGL---cl2---->122GPa	[DM04,VD06,MN06]
ptr/GPa	25 48 97	
Sb	hR2---HGL---HGL---cl2---->65GPa	[MD07,OD09]
ptr/GPa	8.2 9.0 28	
Bi	hR2---mC4---HGL---cl2---->220GPa	[MD07,OD09]
ptr/GPa	2.5 2.7 7.7 oC16HT	

VIA

O	gas---hR2---oF8---mC16---mC16---->132GPa	[FA06,LW06,WD09,KL10]
ptr/GPa	6 8 9 96 mC4 cP16	
S	oF128---hP9---tl16---al6---MG---hR1---->160GPa	[DG05abc]
ptr/GPa	1 29 75 90 155	[MN06,HF06,OD10]
Se	hP3---???---al6---ML---hR1---cl2---->150GPa	[DG05ab,MN06,HF06,OD10]
ptr/GPa	14 23 35 80 140 tl16HT	
Te	hP3---???---al6---ML---cl2---->75GPa	[MH04,DG05,MN06,HF06,OD10]
ptr/GPa	4.0 4.3 4.5 29 hR1HT	
Po	cP1---->0GPa	
ptr/GPa	hR1HT	

VIIA

F	gas---cP16---mC4---->10GPa	
ptr/GPa	2.5 ~20	
Cl	gas---oC8---->45GPa	
ptr/GPa	1	
Br	liquid---oC8---ML---ol2---->125GPa	[KH05]
ptr/GPa	0.2 83 120	
I	oC8---ML---ol2---tl2---cF4---->276GPa	
ptr/GPa	23 25 43 53	

VIIIA

He	gas---hP2---->58GPa	[LL93]
ptr/GPa	12 cl2 cF4	
Ne	gas---cF4---->110GPa	
ptr/GPa	5.1	
Ar	gas---cF4---->77GPa	
ptr/GPa	1.1	
Kr	gas---cF4---hP2---->50GPa	
ptr/GPa	0.93 20	
Xe	gas---cF4---hP2---->236GPa	
ptr/GPa	0.69 20	

IB**Cu** cF4---->236GPa

ptr/GPa

Ag cF4---->236GPa

ptr/GPa

Au cF4----hP2---->275GPa

ptr/GPa 230

[DDC07]

IIB**Zn** hP2---->126GPa

ptr/GPa

Cd hP2---->75GPa

ptr/GPa

Hg hR1----tl2----oP4----hP2---->67GPa

ptr/GPa 4 12 36

[MN08]

IIIB**Sc** hP2----HGL----Sc(III)----Sc(IV)----hP6---->297GPa

ptr/GPa 20 104 140 240

Y hP2----hR3----hP4----cF4---->75GPa

ptr/GPa 13 26 46

[MN08]

IVB**Ti** hP2----hP3---->oC4?----oC4?---->220GPa

ptr/GPa 7 116 140 cl2HT

Zr hP2----hP3----cl2---->75GPa

ptr/GPa 4 32 cl2HT

Hf hP2----hP3----cl2---->252GPa

ptr/GPa 34 71 cl2HT

[MN08]

[VS01_AKB01_JJ02]

VB**V** cl2---->160GPa

ptr/GPa

Nb cl2---->150GPa

ptr/GPa

Ta cl2---->174GPa

ptr/GPa

VIB**Cr** cl2---->10GPa

ptr/GPa

Mo cl2---->272GPa

ptr/GPa

W cl2---->364GPa

ptr/GPa

VII B**Mn** cl58---->190GPa

ptr/GPa cP20HT

Tc hP2---->10GPa

ptr/GPa

Re hP2---->251GPa

ptr/GPa

VIII B

Fe cl2----hP2---->305GPa
ptr/GPa 11 cF4HT
Ru hP2---->25GPa
ptr/GPa
Os hP2---->75GPa
ptr/GPa

[MN08]
[AD13]

IX B

Co hP2-----cF4---->202GPa
ptr/GPa 120
Rh cl2---->56GPa
ptr/GPa
Ir cF4-----hP14---->65GPa
ptr/GPa 59

[MN08]

XB

Ni cF4---->236GPa
ptr/GPa
Pd cF4---->80GPa
ptr/GPa
Pt cF4---->300GPa
ptr/GPa

Ln

La hP4---cF4---hR8---cF4---->70GPa
ptr/GPa 2 7 58 cl2HT
Ce hP4---cF4---cF4---oC4---tl2---->208GPa
ptr/GPa .2 .67 3.9 13 cl2HT
Pr hP4---cF4---hR8---???---oC4---->60GPa
ptr/GPa 4 6.2 10 20 cl2HT
Nd hP4---cF4---hR8---hP3---mC4---oC4---->70GPa
ptr/GPa 5 15 40 75 113 cl2HT
Pm hP4---cF4---hR8---hP3---->60GPa
ptr/GPa 10 18 40
Sm hR3---hP4---cF4---hR8---hP3---tl2---mC4---->70GPa
ptr/GPa 5 15 20 37 75 105 cl2HT
Eu cl2---hP2---ML---???---->92GPa
ptr/GPa 13 31.5 37
Gd hP2---hR3---hP4---cF4---hR8---ml2---->235GPa
ptr/GPa 3.2 7 26 46 61 cl2HT
Tb hP2---hR3---hP4---cF4---hR8---->58GPa
ptr/GPa 3 6 29 32
Dy hP2---hR3---hP4---cF4---hR8---->70GPa
ptr/GPa 5 9 38 40
Ho hP2---hR3---hP4-----hR8---->70GPa
ptr/GPa 10 25 70
Er hP2---hR3---hP4-----hR8---->70GPa
ptr/GPa 12.4 24 67.4
Tm hP2---hR3---hP4---->42GPa
ptr/GPa 10 30
Yb hP2---cF4---cl2---hP2---cF4---hP3---->202GPa
ptr/GPa 0.1 4 30 53 98
Lu hP2---hR3---hP4---cF4---Lu(IV)---->275GPa
ptr/GPa 20 30 88 272

[MK11, HL12]

[TM13]

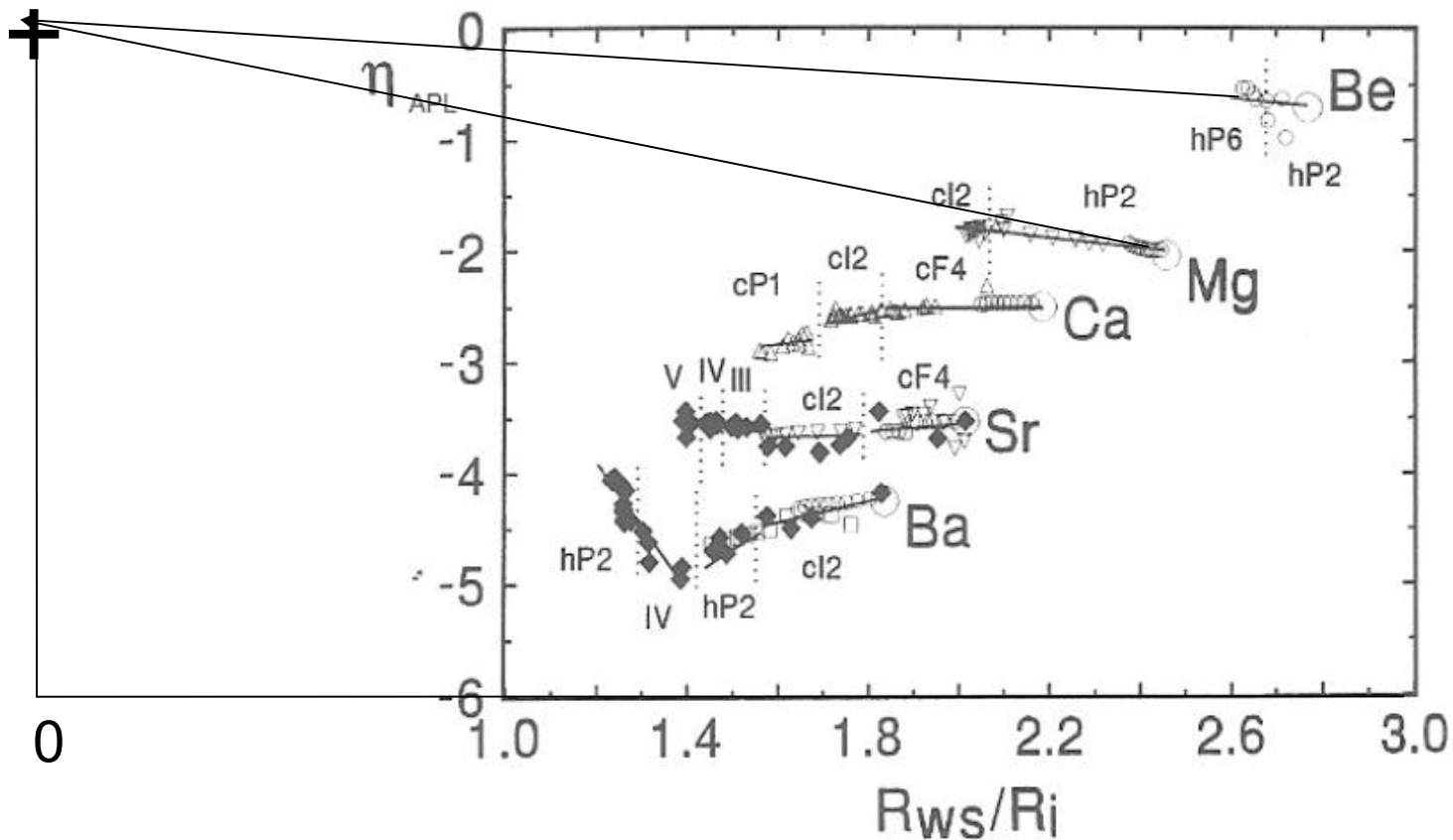


Fig. 17. APL linearization for the EOS data of the alkaline earth metals plotted versus the scale Wigner-Seitz radius ratio R_{WS}/R_i discussed in the text using EOS data from the different sources listed in the original work [7, 37].

"Structural Systematics and Equations of States for the Alkaline Earth Metals under Pressure"
 M. Winzenick and W.B. Holzapfel, p. 384-386 in "High Pressure Science and Technology" ed.
 W. Trzeciakowski, World Scientific, Singapore (1996)

"Physics of Solids under Strong Compression"
 W.B. Holzapfel, Rep. Prog. Phys. 59, 29-90 (1996)

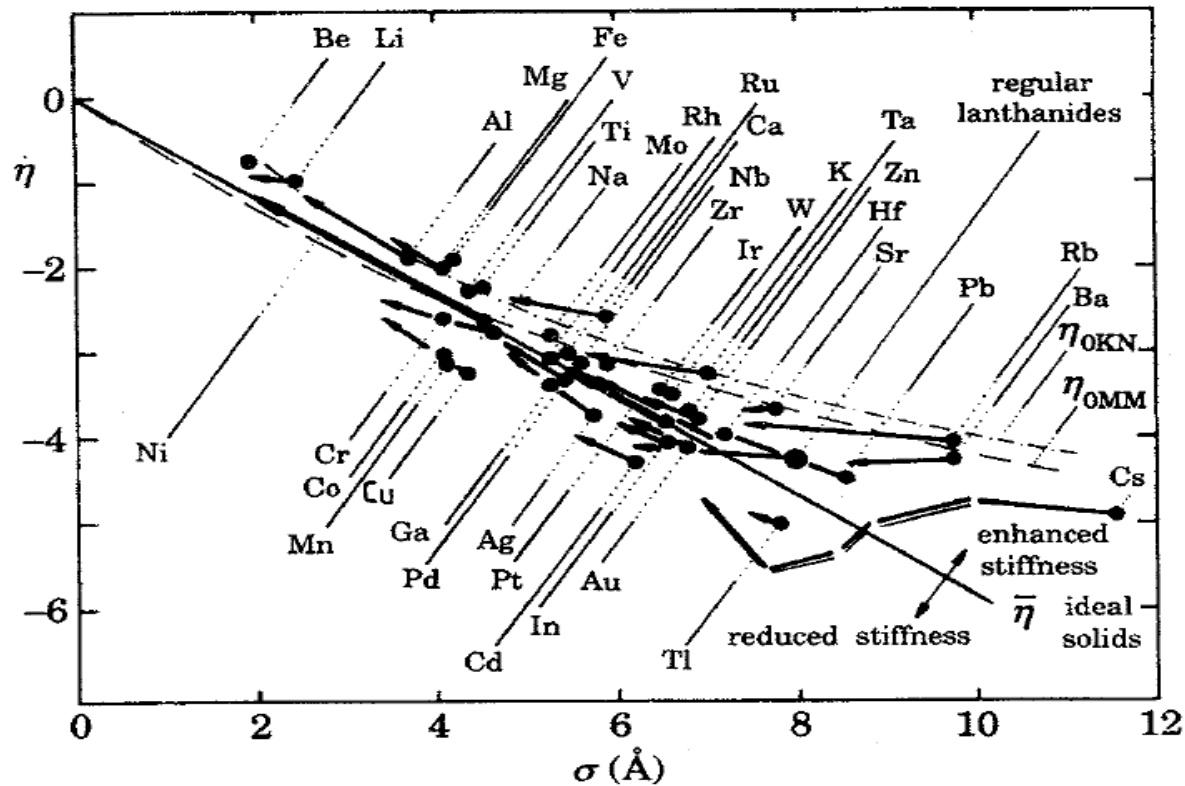


Fig. 1. - EOS data [6, 11-30] for the metallic elements represented in $\eta = \ln(p/p_{FG}) - \ln(1 - (\sigma/\sigma_0))$ vs. σ plots with $\sigma = (ZV \cdot 3/(4\pi))^{1/3}$. The linear correlation η vs. σ , which defines the «ideal» solid behaviour is also compared with earlier correlations between ambient pressure values of K_0 and σ_0 discussed by McMillan [6] and Knopoff [9] and marked with η_{0MM} and η_{0KN} , respectively. Anomalies for the high-pressure phases of Cs are marked by twinned lines.

"Equations of State for Ideal and Real Solids under Strong Compression"
W.B. Holzapfel, Europhys. Lett. 16, 67-72 (1991)

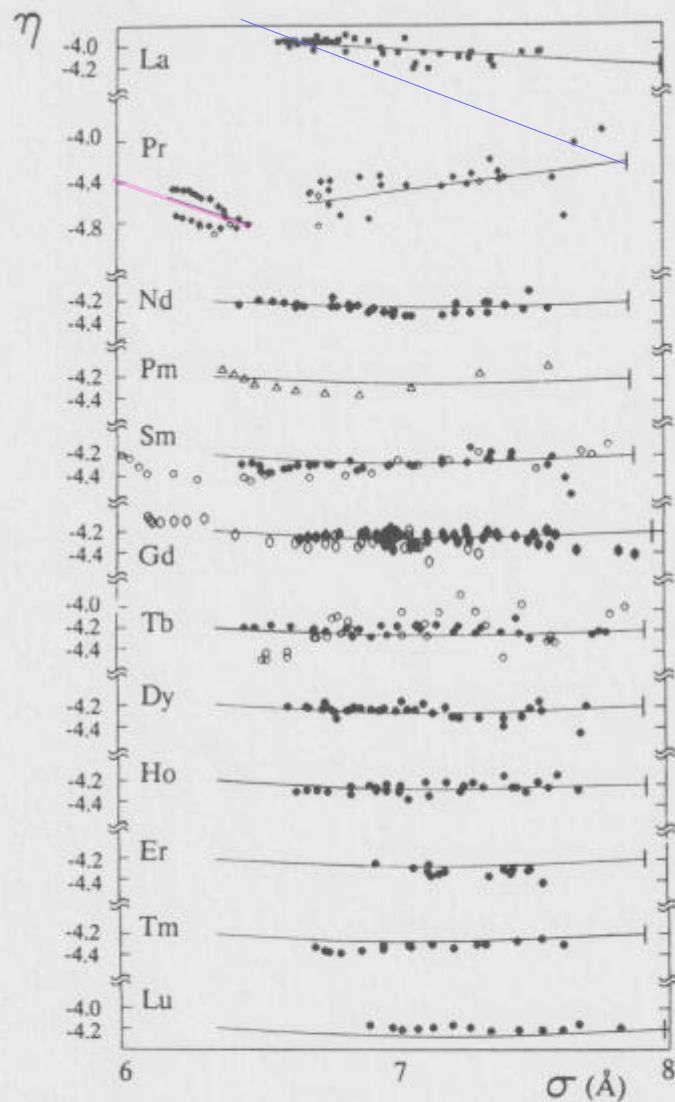


FIG. 16. EOS data for the "regular" lanthanides in η - σ representation with $\eta = \ln(p/p_{FG}) - \ln(1 - \sigma/\sigma_0)$ using Thomas-Fermi scaling for the atomic length parameter σ and the Fermi gas pressure p_{FG} . Open symbols refer to recent data from the literature (Refs. 14–23) for this extended pressure range.

"Atomic Volumes for Rare Earth Metals under Pressure to 40 GPa and Above"
W. A. Grosshans and W.B. Holzapfel,
Phys. Rev. B 45, 5171-5178 (1992)

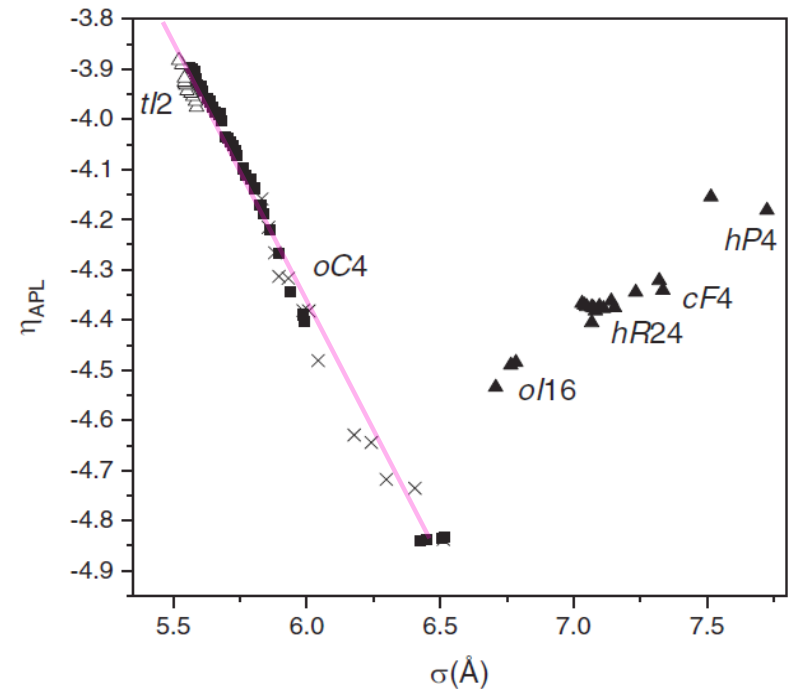


FIG. 7. Linearization of the compression of Pr shown in the form of an η_{APL} - σ plot, where $\sigma = \sigma_0 x$. The data from the lower-pressure phases (*hP4*, *cF4*, *hR24*, and *oI16*) are plotted with filled triangles, while our data from *oC4*-Pr are plotted with filled squares and the *oC4*-Pr data from the study of Chesnut and Vohra [29] are shown as crosses. For clarity, the current data for *tI2*-Pr are plotted with unfilled triangles.

— Simple 1. order AP1-EOS

High-pressure structure of praseodymium revisited:
In search of a uniform structural phase sequence for
the lanthanide elements

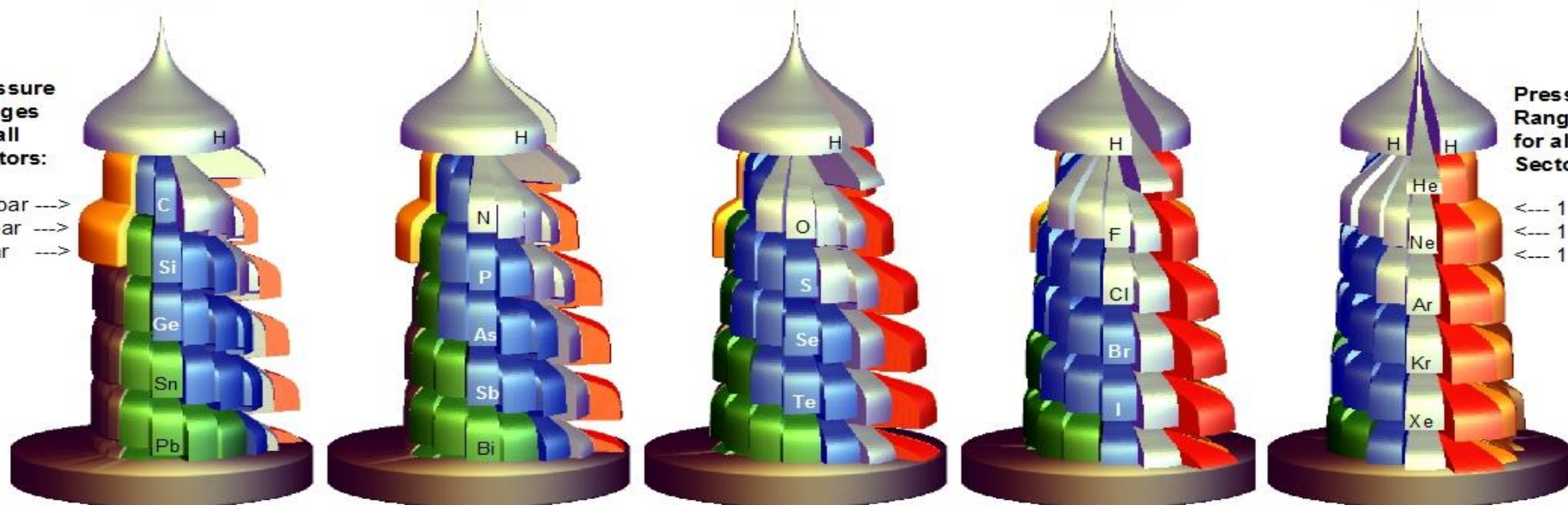
S.E. Finnegan, M.G. Stevenson, E.J. Pace, C.V.
Storm, J.D. McHardy, M.I. McMahon, S.G.
MacLeod, E. Plekhanov, N. Bonini, C. Weber, *Phys.*
Rev. B **105**, 174101 (2022)

The fascinating World of the Elements under Pressure



Pressure Ranges for all Sectors:

1 Mbar --->
1 kbar --->
1 bar --->



Pressure Ranges for all Sectors:

<--- 1 Mbar
<--- 1 kbar
<--- 1 bar

Model for a sculpture to be decorated with the colourful phase diagrams.
In honour of Aristoteles (†322 B.C.) and Galilei (†1642 A.D.) founders of modern science proclaiming:

***Measure all you can measure
and what you can't, make it measurable !***



United States of the Elements – USE

At the beginning there was a big bang, which generated the Hydrogen and little Helium, that is true, was in this early stardust brew.

Some dust condensed by gravity and stars appeared with density just high enough for the ignition of nuclear fusion with the provision

for many more new elements, but these were not the final ends!

The heavy ones had still to wait for supernovae, which came late as star explosions, an event, which is considered as the end of all the element creation, we only miss still the equation

explaining how the numbers came to fit all this! This is the game!

With all the elements now here, some order makes this world more clear. Wise man produced a Periodic Table with 8 Main Groups which do enable

to show some common properties in 8 columns, but there are these remaining elements between with 10 at first and then 14,

Transition Metals, 3 rows of 10, and Lanthanoides, with 14 then.

The Actinoides, we will not need, they are unstable, well indeed!-

And still more order is present, if you look carefully at the end!

You can first see right on the top the Hydrogen and if you stop,

you see for Helium a slit just wide enough to give a fit for the Rare Gases as column on top with our Helium.

The other columns broad and wide include the Main Groups not so tide as all the lower sections squeezed between for the Transition Metals in this scheme.

And in the column number 3 the Rare Earth Metals you can see.

The chemists now look for reactions. The physicists see other actions!

They change the temperature and pressure and keep in mind, they have to measure

the properties in all these states and some results lead to debates before one reaches the consensus on these results, which are immense

in these domains, which reach as far, as the interior of some star!

Much more ideas have been cast into this figure, but at last

a book can only give to you for this artwork the final clue!

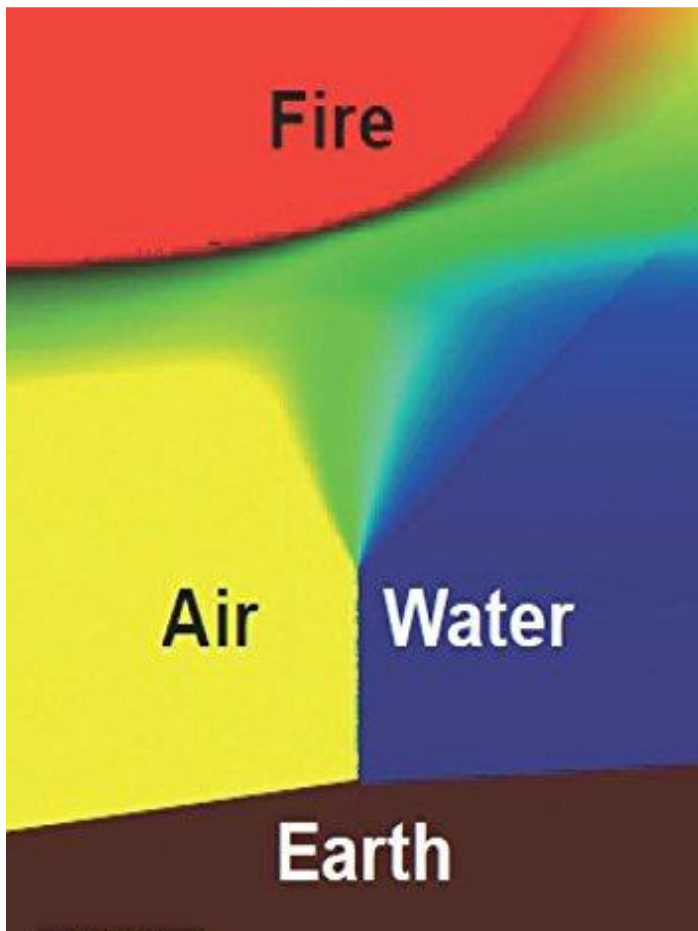
Colorful systematic in the phase-diagrams of the elements

A simple guide to the world of high pressure

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Intention: stimulate young scientists to look at structural changes in matter
in wide fields of pressure and temperature

4 essentia 4 classical elements 4 forms of being for matter



states of matter
in wide ranges
of
temperature
and
pressure

