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Understanding Atoms in Tight Places

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Department of Chemistry and Chemical Engineering
Division of Chemistry and Biochemistry
Chalmers University of Technology

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rahmlab.com

CEST Skolkovo
July 8th 2021

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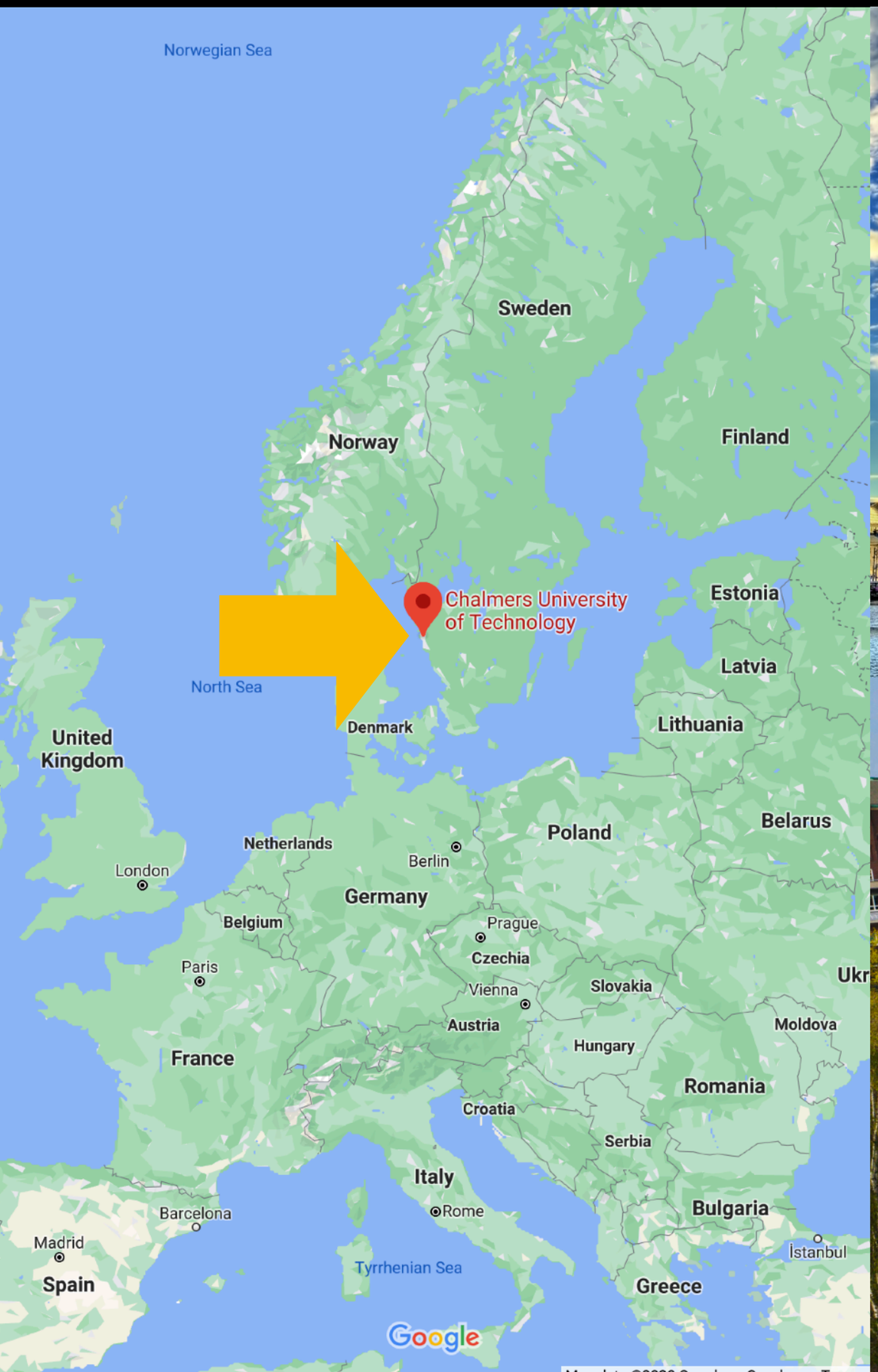

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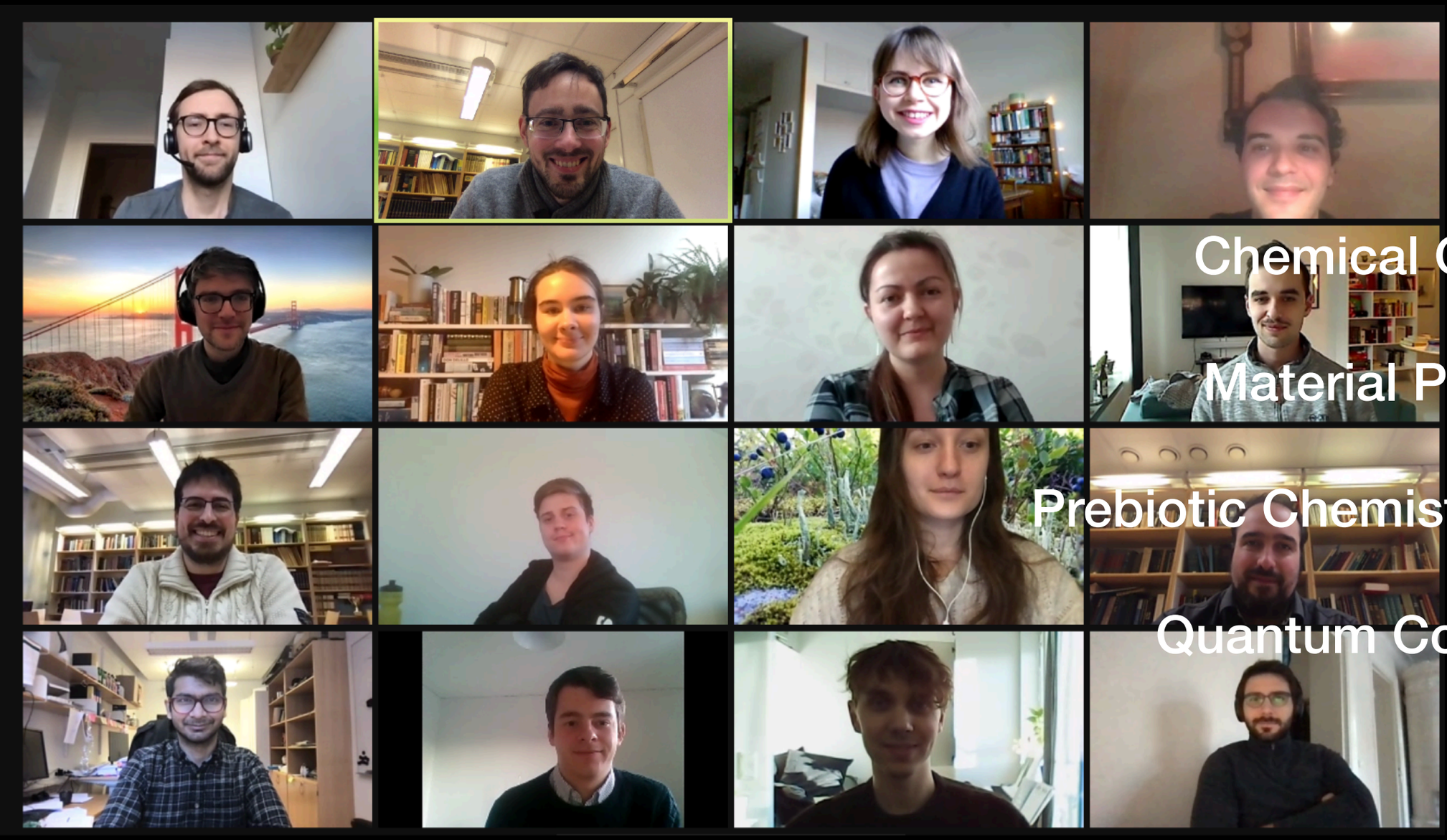
The Research Group



Chemical Concepts

Material Prediction

Prebiotic Chemistry/Astrobiology

Quantum Computation

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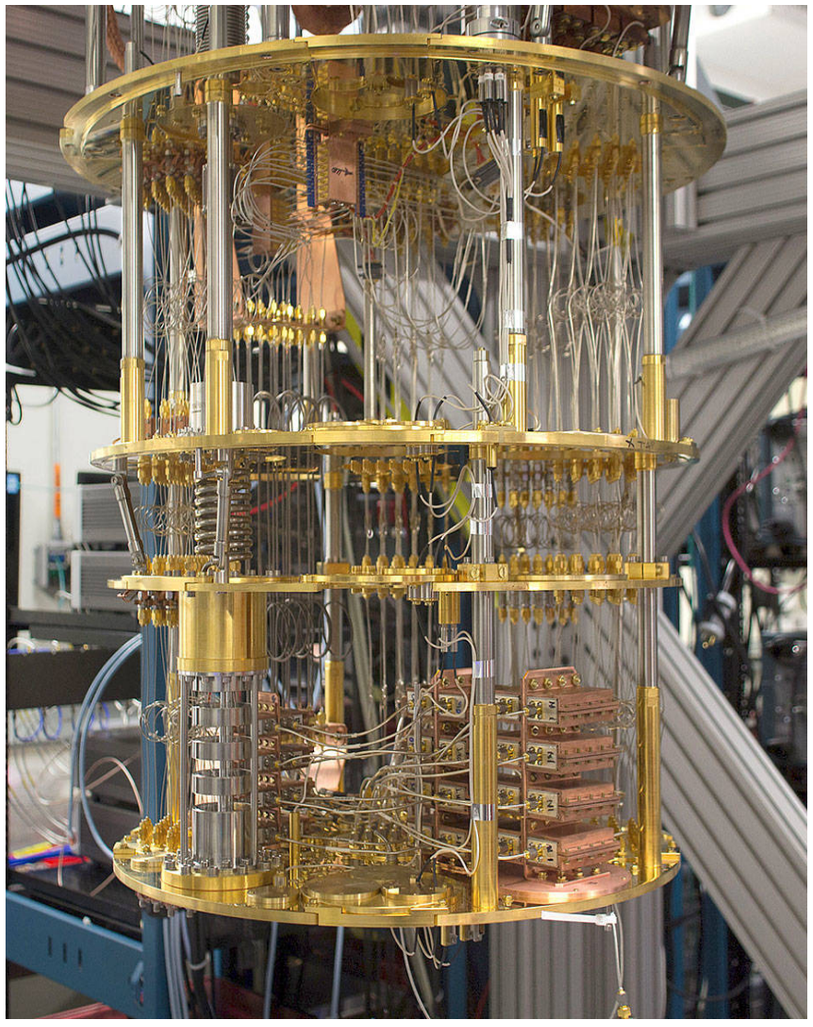
WACQT | Wallenberg Centre for Quantum Technology

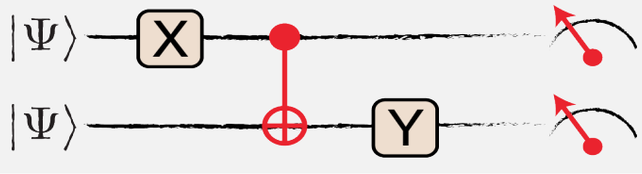


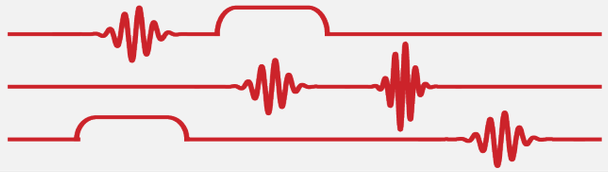
A full-stack approach at Chalmers along two tracks: discrete and continuous variables implemented with superconducting circuits

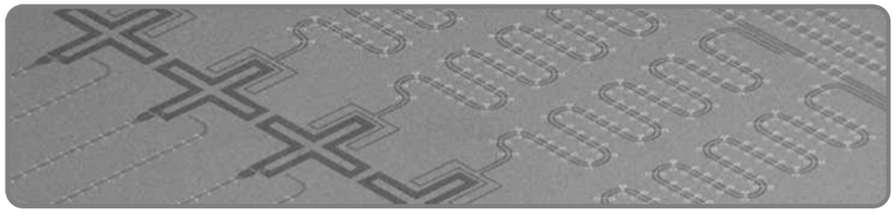
Now scaling up after having demonstrated the basic building blocks

20 qubits this year
100 qubits after 10 years

```
let shorCorrector (qs:Qubits) =
    let out = xflipSyndrome qs.[0 .. 2]
    if (out > 0) then
        X [qs.[out - 1]]
```







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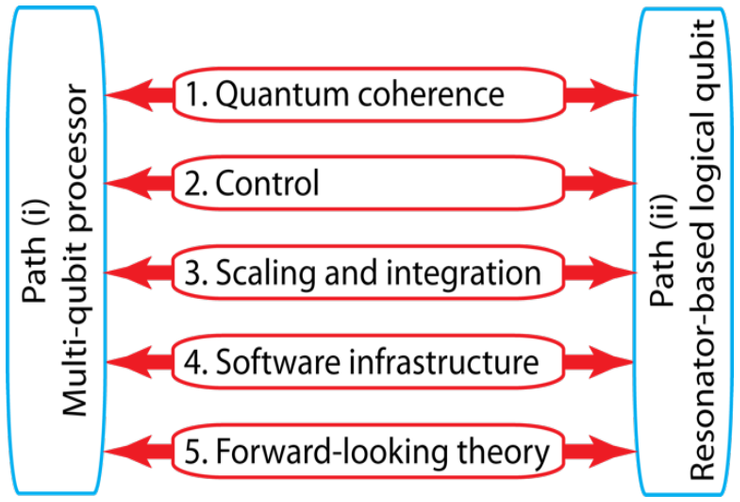
The WACQT team

Strong collaboration between experiment and theory to tackle the challenges at all levels of the stack

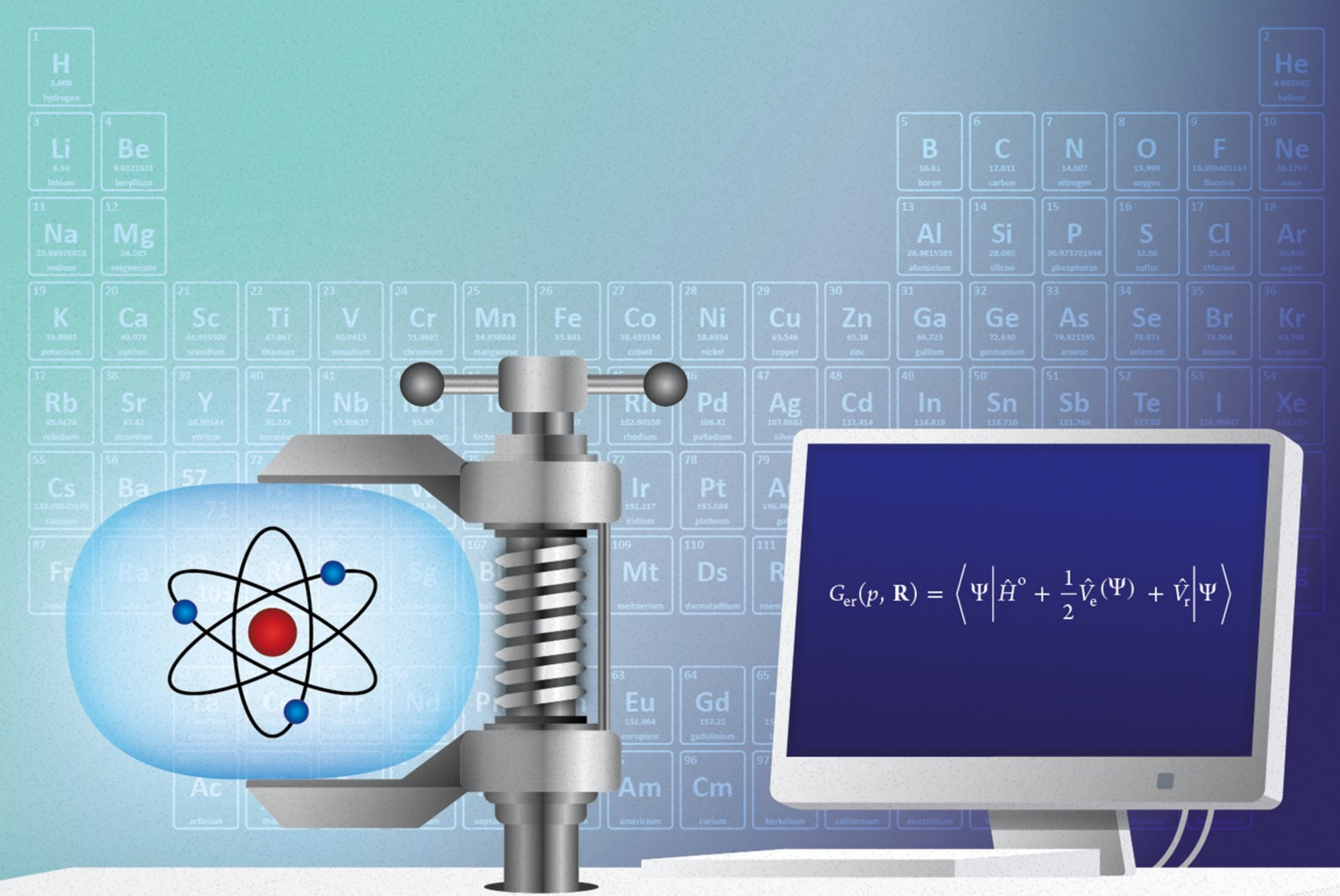
50 people gathered pre-covid: physicists, chemists, computer scientists, industrial PhD students

”Work with us”

WACQT will hire 40 more people 2021-2022
>15 positions open now (postdocs, researchers, PhD students)



www.wacqt.se


$G_{er}(p, \mathbf{R}) = \left\langle \Psi \middle| \hat{H}^{o} + \frac{1}{2}\hat{V}_{e}(\Psi) + \hat{V}_{r} \middle| \Psi \right\rangle$

Collaborators & Acknowledgements

Roald Hoffmann
Cornell

Toby Zeng
York University

Roberto Cammi
University of Parma

Neil Ashcroft
Cornell

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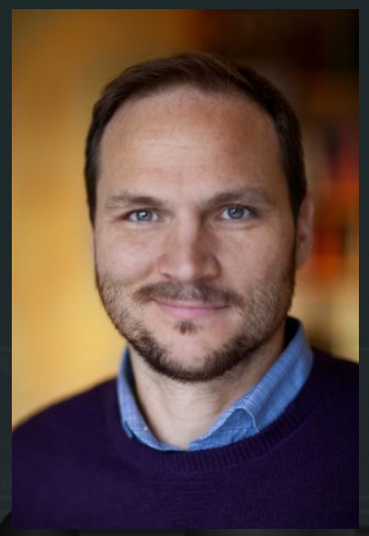
Funding

Collaborators & Acknowledgements

Paul Erhart
Chalmers



Magnus Rahm
Chalmers

Mattias Ångqvist
Chalmers

$$G_{er}(p, \mathbf{R}) = \left\langle \Psi \middle| \hat{H}^{\circ} + \frac{1}{2}\hat{V}_{e}(\Psi) + \hat{V}_{r} \middle| \Psi \right\rangle$$

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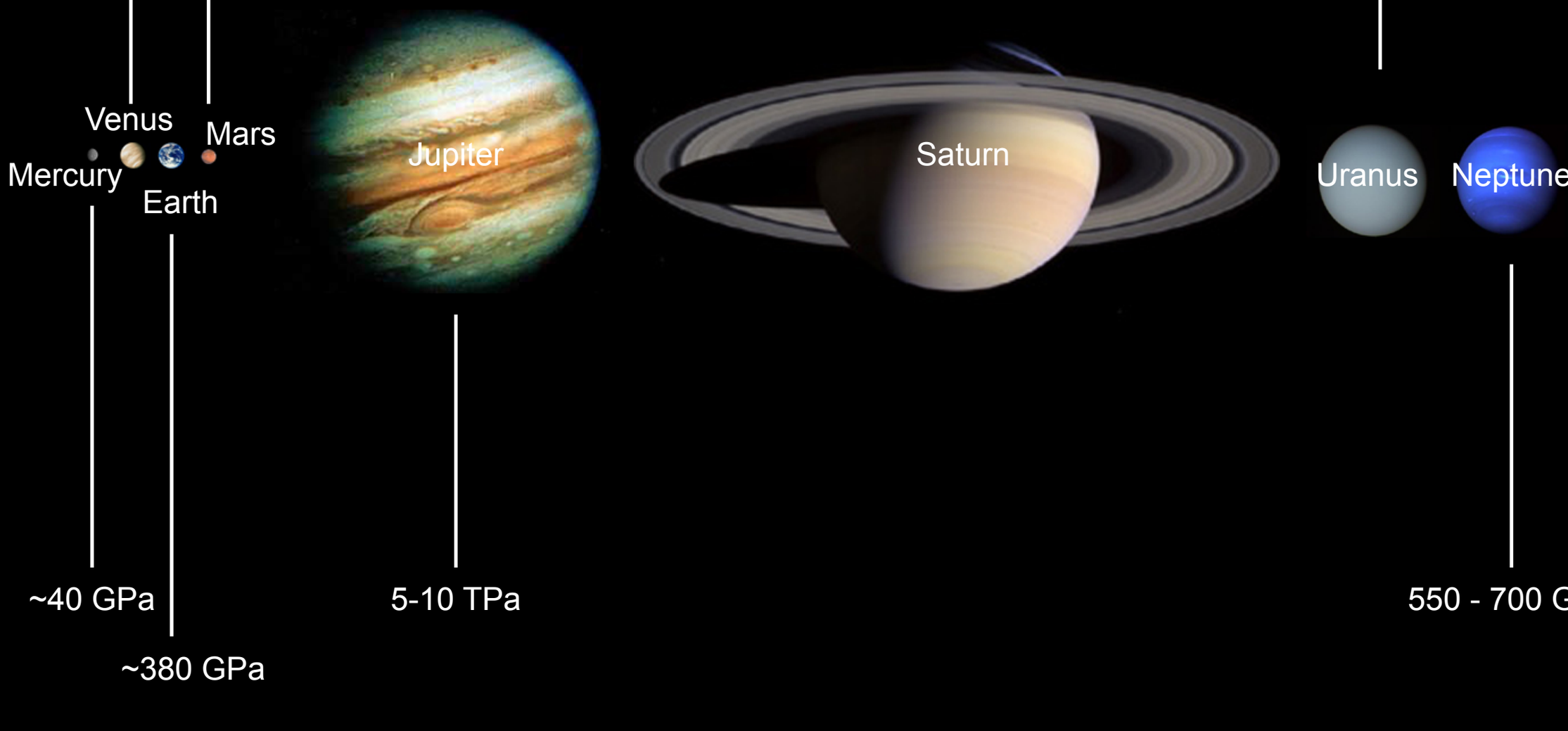
High Pressure Chemistry

~40 GPa

~290 GPa

500 - 800 GPa

400 - 550 GPa

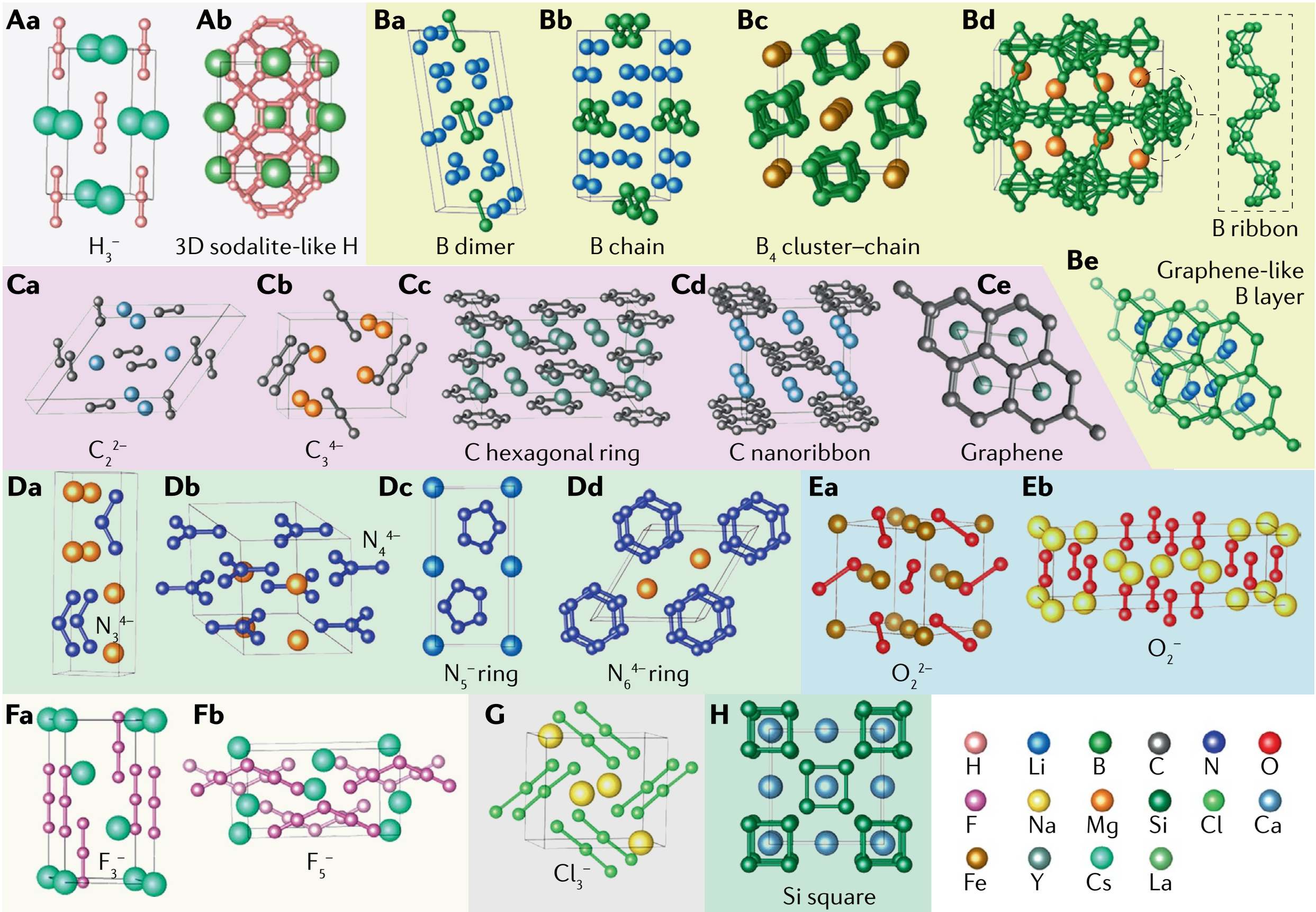


~40 GPa

~380 GPa

5-10 TPa

550 - 700 GPa



M. Miao, Y. Sun, E. Zurek, H. Lin, Nat. Rev. 2020

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Electronegativity of the Atoms

Average valence electron binding energy as T → 0K

eV e^{-1}

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ 13.6																	He $1s^2$ 24.6
2	Li $2s^1$ 5.4	Be $2s^2$ 9.3											B $2s^22p^1$ 11.4	C $2s^22p^2$ 13.9	N $2s^22p^3$ 16.9	O $2s^22p^4$ 18.6	F $2s^22p^5$ 23.3	Ne $2s^22p^6$ 28.3
3	Na $3s^1$ 5.1	Mg $3s^2$ 7.6											Al $3s^23p^1$ 9.1	Si $3s^23p^2$ 10.8	P $3s^23p^3$ 12.8	S $3s^23p^4$ 13.6	Cl $3s^23p^5$ 16.3	Ar $3s^23p^6$ 19.1
4	K $4s^1$ 4.3	Ca $4s^2$ 6.1	Sc $4s^23d^1$ 7.0	Ti $4s^23d^2$ 8.4	V $4s^23d^3$ 9.7	Cr $4s^13d^5$ 8.0	Mn $4s^23d^5$ 12.3	Fe $4s^23d^6$ 10.1	Co $4s^23d^7$ 11.9	Ni $4s^23d^8$ 12.9	Cu $4s^13d^{10}$ 10.2	Zn $4s^23d^{10}$ 15.9	Ga $4s^24p^1$ 9.9	Ge $4s^24p^2$ 11.1	As $4s^24p^3$ 12.5	Se $4s^24p^4$ 13.2	Br $4s^24p^5$ 15.2	Kr $4s^24p^6$ 17.4
5	Rb $5s^1$ 4.2	Sr $5s^2$ 5.7	Y $5s^24d^1$ 6.3	Zr $5s^24d^2$ 7.5	Nb $5s^14d^4$ 7.0	Mo $5s^14d^5$ 8.3	Tc $5s^24d^5$ 10.9	Ru $5s^14d^7$ 8.4	Rh $5s^14d^8$ 9.3	Pd $4d^{10}$ 8.3	Ag $5s^14d^{10}$ 12.0	Cd $5s^24d^{10}$ 16.1	In $5s^25p^1$ 9.3	Sn $5s^25p^2$ 10.2	Sb $5s^25p^3$ 11.2	Te $5s^25p^4$ 12.0	I $5s^25p^5$ 13.4	Xe $5s^25p^6$ 14.9
6	Cs $6s^1$ 3.9	Ba $6s^2$ 5.2	Lu $6s^25d^1$ 6.4	Hf $6s^25d^2$ 7.1	Ta $6s^25d^3$ 7.8	W $6s^25d^4$ 8.6	Re $6s^25d^5$ 9.1	Os $6s^25d^6$ 9.2	Ir $6s^25d^7$ 10.8	Pt $6s^15d^9$ 9.5	Au $6s^15d^{10}$ 10.9	Hg $6s^25d^{10}$ 14.1	Tl $6s^26p^1$ 10.2	Pb $6s^26p^2$ 11.0	Bi $6s^26p^3$ 10.7	Po $6s^26p^4$ 12.2	At $6s^26p^5$ 12.6	Rn $6s^26p^6$ 14.6
7	Fr $7s^1$ 4.1	Ra $7s^2$ 5.3																
6			La $6s^25d^1$ 6.0	Ce $6s^24f^15d^1$ 7.3	Pr $6s^24f^3$ 6.7	Nd $6s^24f^4$ 7.2	Pm $6s^24f^5$ 7.4	Sm $6s^24f^6$ 8.3	Eu $6s^24f^7$ 9.4	Gd $6s^24f^75d^1$ 13.8	Tb $6s^24f^9$ 7.7	Dy $6s^24f^{10}$ 8.4	Ho $6s^24f^{11}$ 8.3	Er $6s^24f^{12}$ 7.6	Tm $6s^24f^{13}$ 9.0	Yb $6s^24f^{14}$ 10.2	
7			Ac $7s^26d^1$ 5.8	Th $7s^26d^2$ 6.4	Pa $7s^25f^26d^1$ 6.3	U $7s^25f^36d^1$ 7.5	Np $7s^25f^46d^1$ 8.2	Pu $7s^25f^6$ 7.3	Am $7s^25f^7$ 8.3	Cm $7s^25f^76d^1$ 10.9								

Element
ground state valence configuration
$\bar{\chi}$

1 Pauling unit ≈ 6 eV e^{-1}

Rahm, M., Zeng, T., Hoffmann, R., J. Am. Chem. Soc., 141, 342-351, 2019

Experimental and/or GMC-QDPT+ORMAS+SOC/ANO-RCC

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Element
ground state
valence
configuration
χ

Rahm, M., Zeng, T., R. Hoffmann, J. Am. Chem. Soc., 141, 342-351, 2019

Experimental and/or GMC-QDPT+ORMAS+SOC/ANO-RCC

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Article

Cite This: J. Am. Chem. Soc. 2019, 141, 10253−10271

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Squeezing All Elements in the Periodic Table: Electron Configuration and Electronegativity of the Atoms under Compression

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§Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853, United States
∥Department of Chemistry and Chemical Biology, Baker Laboratory, Cornell University, Ithaca, New York 14853, United States

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Non-bonded Radii of the Atoms Under Compression

Martin Rahm ✉, Mattias Ångqvist, J. Magnus Rahm, Paul Erhart, Roberto Cammi

First published: 08 September 2020 | https://doi.org/10.1002/cphc.202000624

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Atomic and Ionic Radii of Elements 1–96

Dr. Martin Rahm ✉, Prof. Dr. Roald Hoffmann ✉, Prof. Dr. N. W. Ashcroft

First published: 24 August 2016 Full publication history

DOI: 10.1002/chem.201602949 View/save citation

1 H 1.54 Hydrogen																	2 He 1.34 Helium
3 Li 2.20 Lithium	4 Be 2.19 Beryllium											5 B 2.05 Boron	6 C 1.90 Carbon	7 N 1.79 Nitrogen	8 O 1.71 Oxygen	9 F 1.63 Fluorine	10 Ne 1.56 Neon
11 Na 2.25 Sodium	12 Mg 2.40 Magnesium											13 Al 2.39 Aluminum	14 Si 2.32 Silicon	15 P 2.23 Phosphorus	16 S 2.14 Sulfur	17 Cl 2.06 Chlorine	18 Ar 1.97 Argon
19 K 2.34 Potassium	20 Ca 2.70 Calcium	21 Sc 2.63 Scandium	22 Ti 2.57 Titanium	23 V 2.52 Vanadium	24 Cr 2.33 Chromium	25 Mn 2.42 Manganese	26 Fe 2.37 Iron	27 Co 2.33 Cobalt	28 Ni 2.29 Nickel	29 Cu 2.17 Copper	30 Zn 2.22 Zinc	31 Ga 2.33 Gallium	32 Ge 2.34 Germanium	33 As 2.31 Arsenic	34 Se 2.24 Selenium	35 Br 2.19 Bromine	36 Kr 2.12 Krypton
37 Rb 2.40 Rubidium	38 Sr 2.79 Strontium	39 Y 2.74 Yttrium	40 Zr 2.69 Zirconium	41 Nb 2.51 Niobium	42 Mo 2.44 Molybdenum	43 Tc 2.52 Technetium	44 Ru 2.37 Ruthenium	45 Rh 2.33 Rhodium	46 Pd 2.15 Palladium	47 Ag 2.25 Silver	48 Cd 2.38 Cadmium	49 In 2.46 Indium	50 Sn 2.48 Tin	51 Sb 2.46 Antimony	52 Te 2.42 Tellurium	53 I 2.38 Iodine	54 Xe 2.32 Xenon
55 Cs 2.49 Cesium	56 Ba 2.93 Barium		72 Hf 2.64 Hafnium	73 Ta 2.58 Tantalum	74 W 2.53 Tungsten	75 Re 2.49 Rhenium	76 Os 2.44 Osmium	77 Ir 2.40 Iridium	78 Pt 2.30 Platinum	79 Au 2.26 Gold	80 Hg 2.29 Mercury	81 Tl 2.42 Thallium	82 Pb 2.49 Lead	83 Bi 2.50 Bismuth	84 Po 2.50 Polonium	85 At 2.47 Astatine	86 Rn 2.43 Radon
87 Fr 2.58 Francium	88 Ra 2.92 Radium																
			57 La 2.84 Lanthanum	58 Ce 2.82 Cerium	59 Pr 2.86 Praseodymium	60 Nd 2.84 Neodymium	61 Pm 2.83 Promethium	62 Sm 2.80 Samarium	63 Eu 2.80 Europium	64 Gd 2.77 Gadolinium	65 Tb 2.76 Terbium	66 Dy 2.75 Dysprosium	67 Ho 2.73 Holmium	68 Er 2.72 Erbium	69 Tm 2.71 Thulium	70 Yb 2.77 Ytterbium	71 Lu 2.70 Lutetium
			89 Ac 2.93 Actinium	90 Th 2.88 Thorium	91 Pa 2.85 Protactinium	92 U 2.83 Uranium	93 Np 2.81 Neptunium	94 Pu 2.78 Plutonium	95 Am 2.76 Americium	96 Cm 2.64 Curium							

1.3 Å

2.9 Å

Rahm, M.; Hoffmann, R.; Ashcroft, N. W. Chem. Eur. J. 22, 14625-14632, 2016

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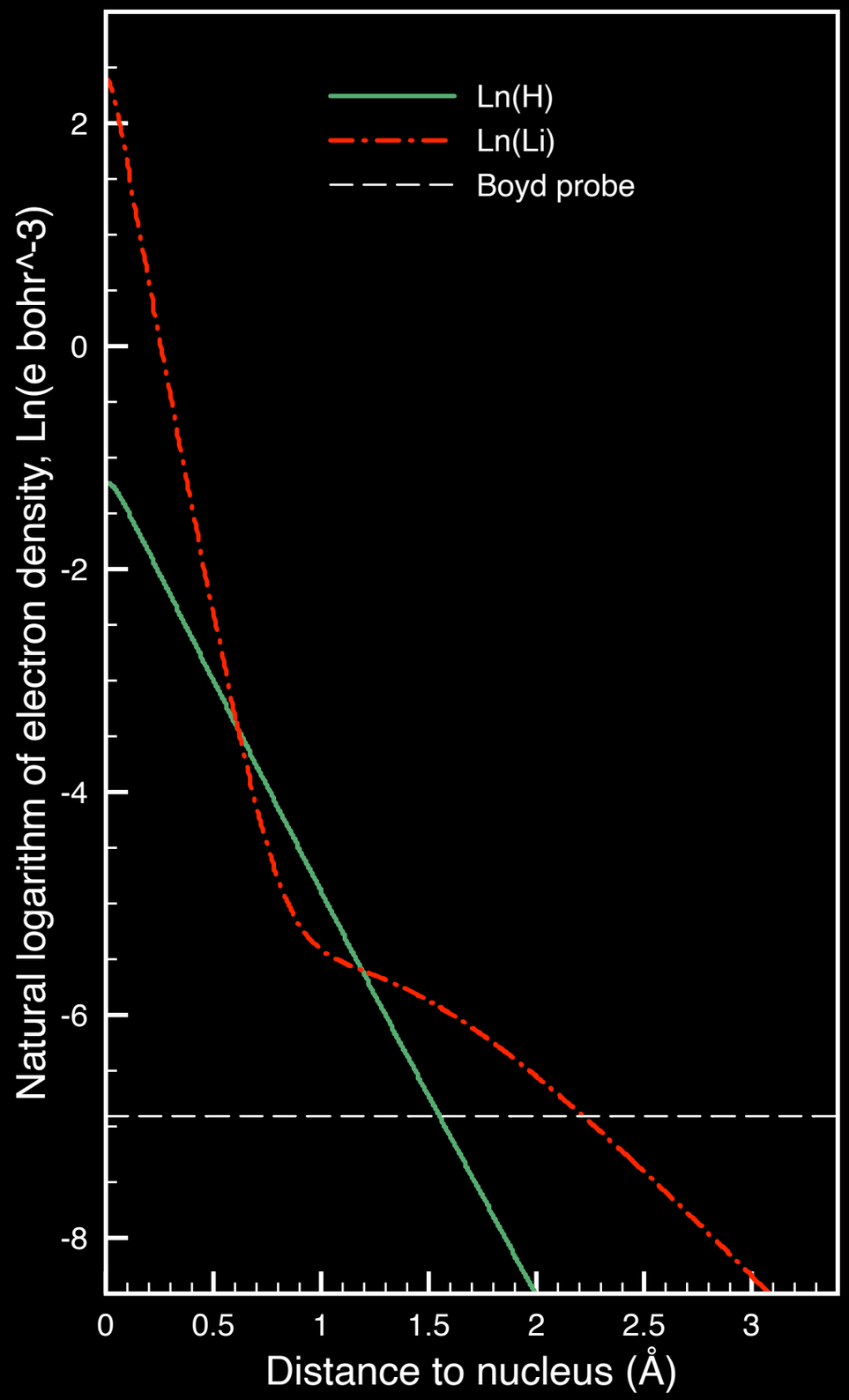
radii defined from:
0.001 e bohr^{-3} electron density cutoff.



Rahm, M.; Hoffmann, R.; Ashcroft, N. W. Chem. Eur. J. 22, 14625-14632, 2016

The Compression Model

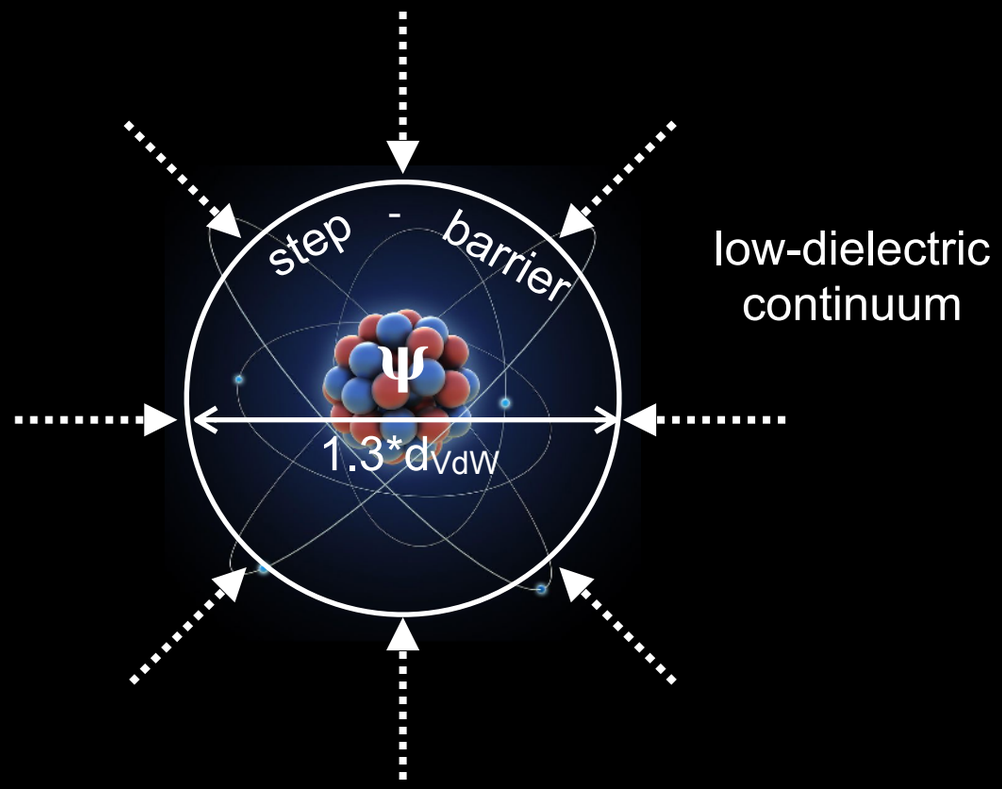
unperturbed atom

$$G = \left\langle \Psi \middle| \hat{H}^0 + \frac{1}{2}\hat{V}_e(\Psi) + \hat{V}_r(\Psi) \middle| \Psi \right\rangle$$

electrostatic and Pauli repulsion with external continuum

- Hybrid DFT (PBE0)
- Relativistic Hamiltonian (DKH2)
- Very large basis set (ANO-RCC)

$$P = \frac{\delta G}{\delta V_c}$$



Wigner, E.; Seitz, F. *Phys. Rev.* 43, 804-810, **1933**
Michels, A.; de Boer, J.; Bijl, A., *Physica*, 4, 981-994, **1937**
Sen, K. D. *Electronic Structure of Quantum Confined Atoms and Molecules*, Springer, **2014**
Cammi, R.; Chen, B.; Rahm, M. *J. Comp. Chem.* 39, 2243-2250, **2018**

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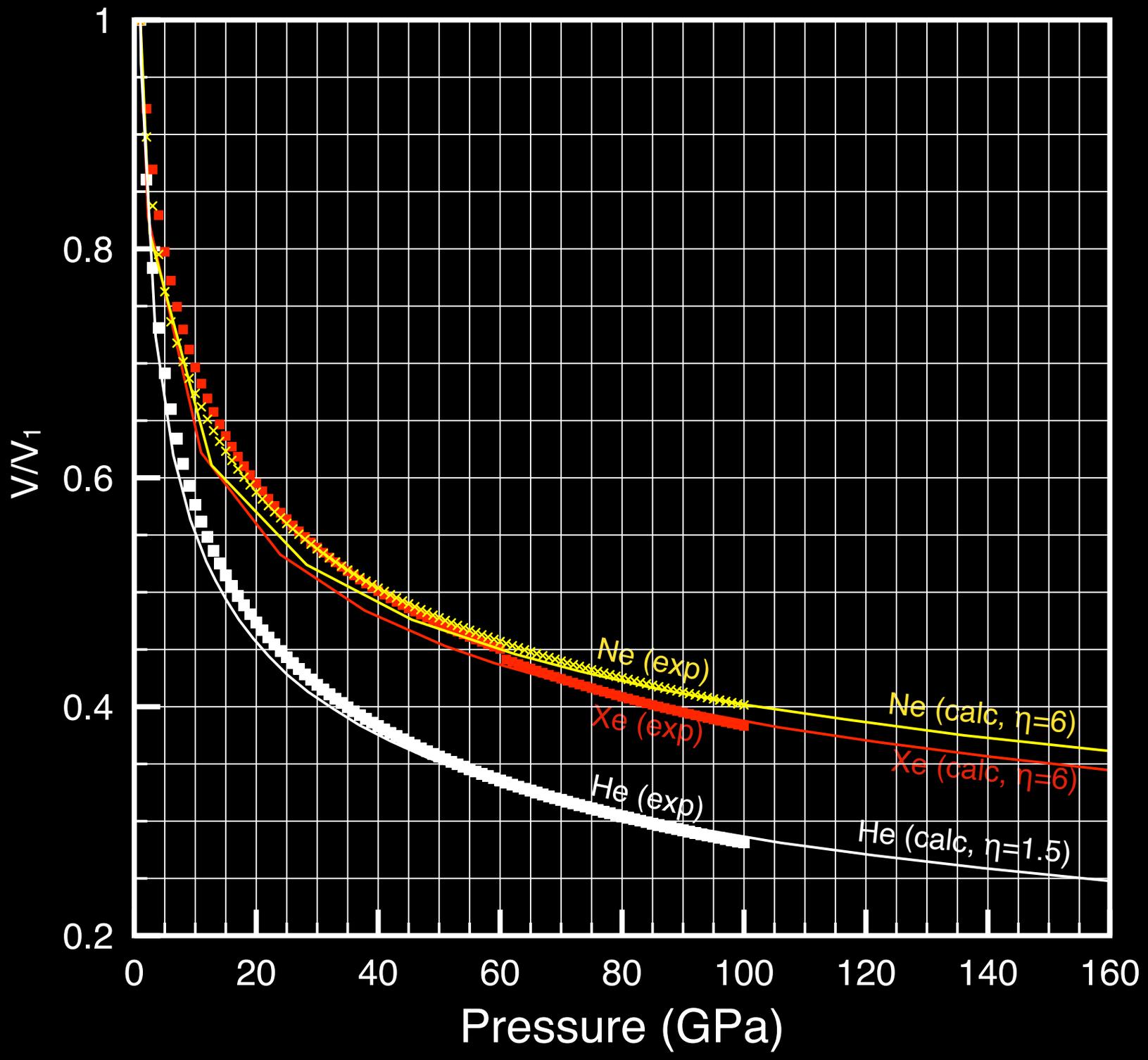
Method Validation



Rahm, M., Cammi, R., N. W. Ashcroft, R. Hoffmann, *J. Am. Chem. Soc.*, 141, 10253-10271, 2019

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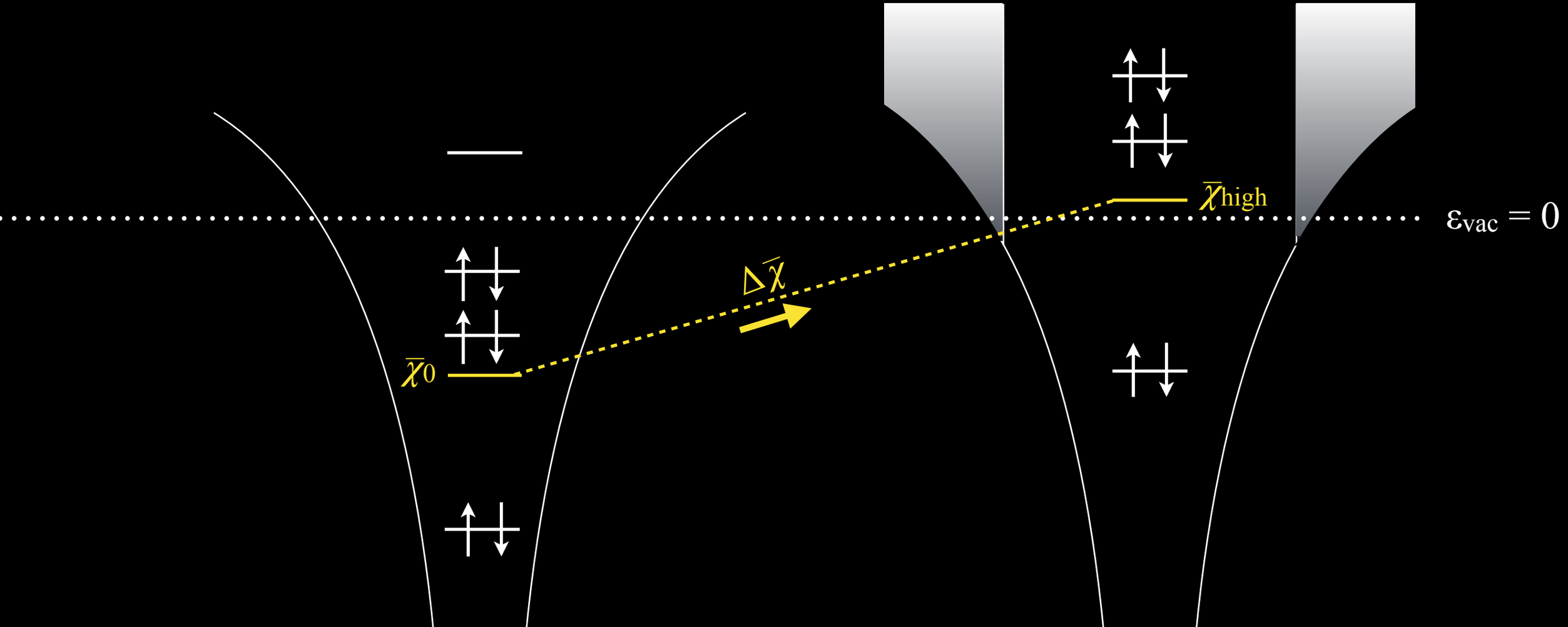
What happens when an atom is compressed?

low pressure

high pressure



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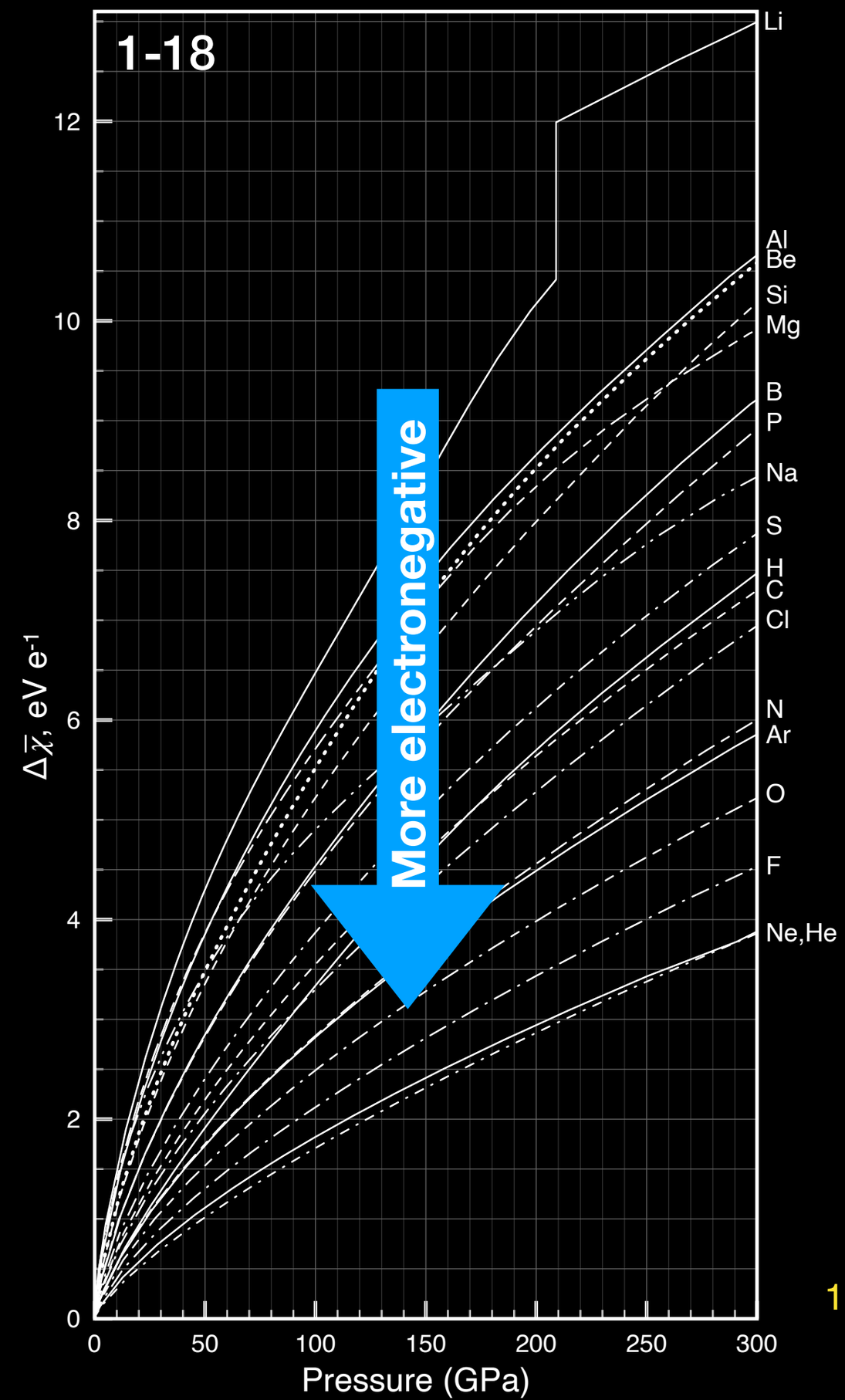
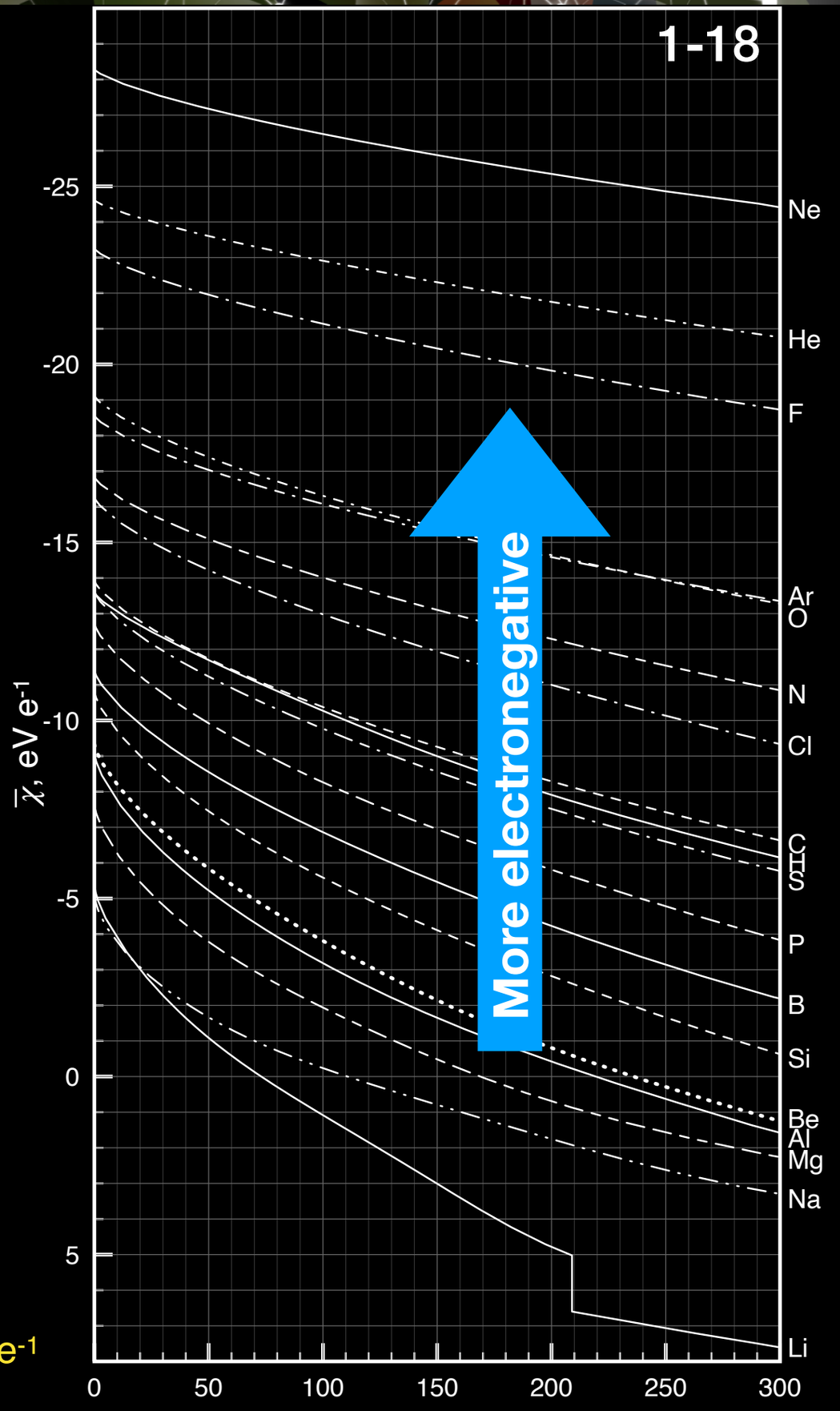


$\Delta\bar{\chi}$ - $\bar{\chi}_{1atm}$

1 Pauling unit ≈ 6 eV e^{-1}



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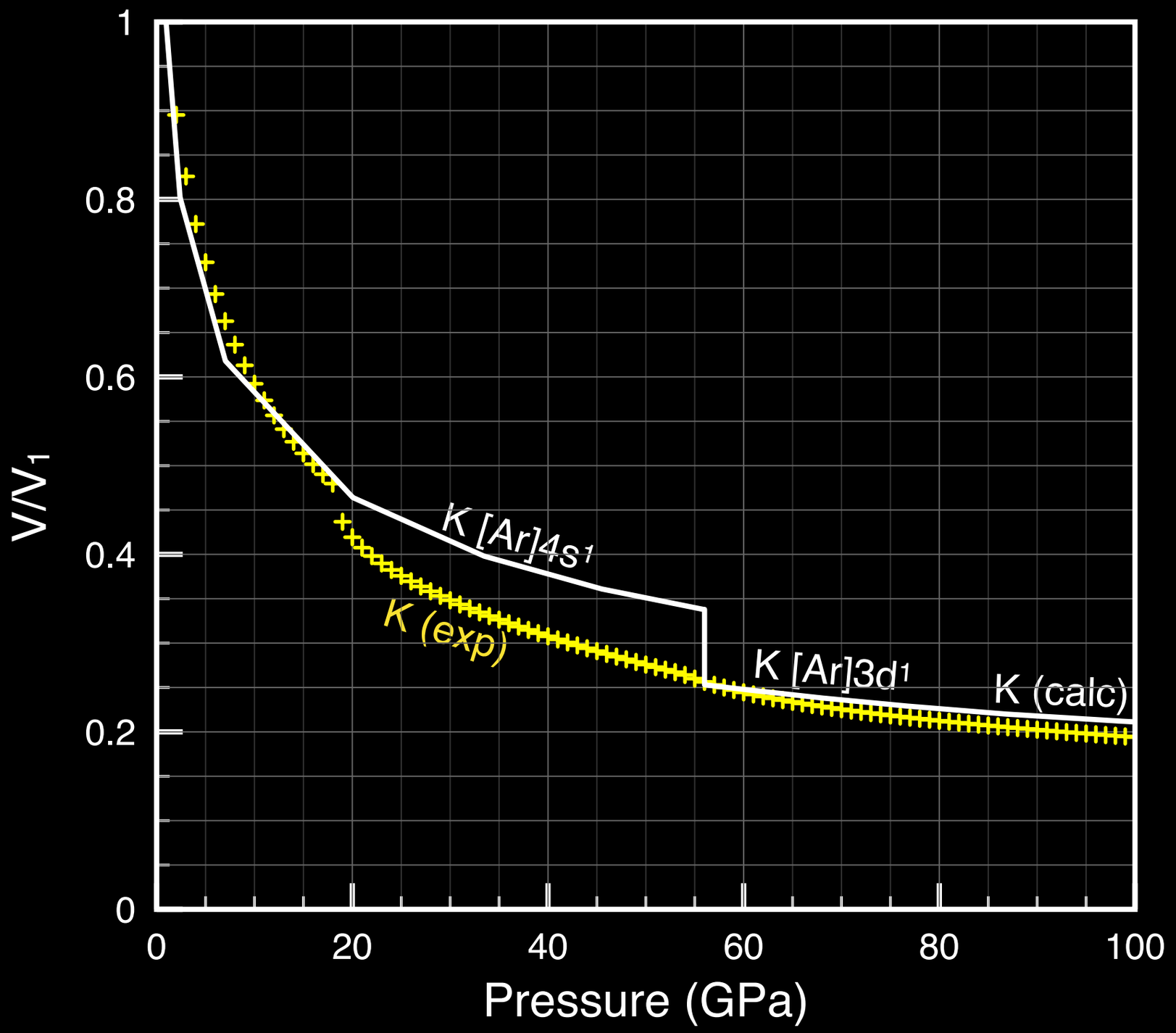

Young, D. A., Cynn, H., Söderlind, P., Landa, A., *Phys. Chem. Ref. Data*, 45, 043101, 2016.
Rahm, M., Cammi, R., N. W. Ashcroft, R. Hoffmann, *J. Am. Chem. Soc.*, 141, 10253-10271, 2019

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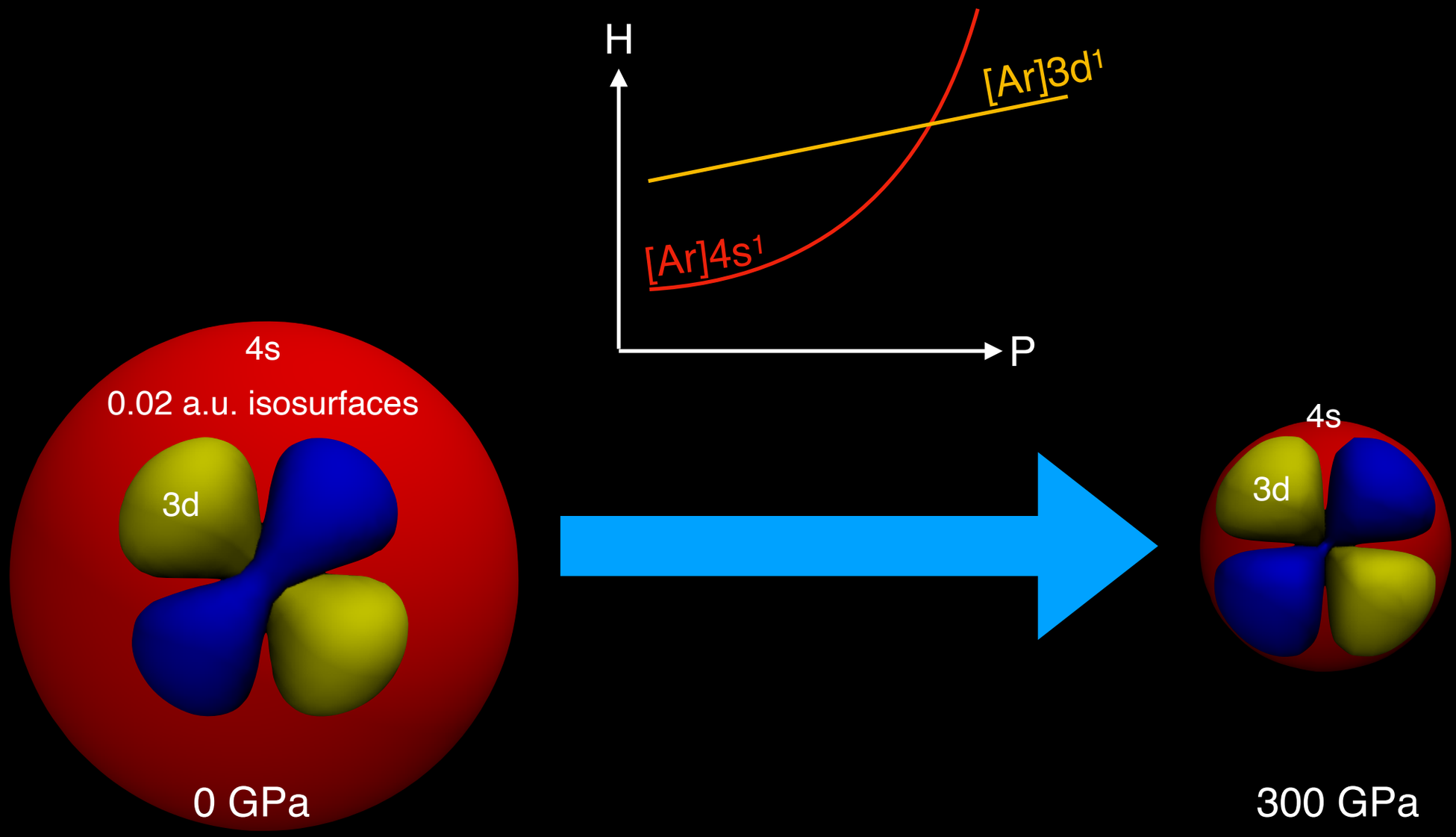
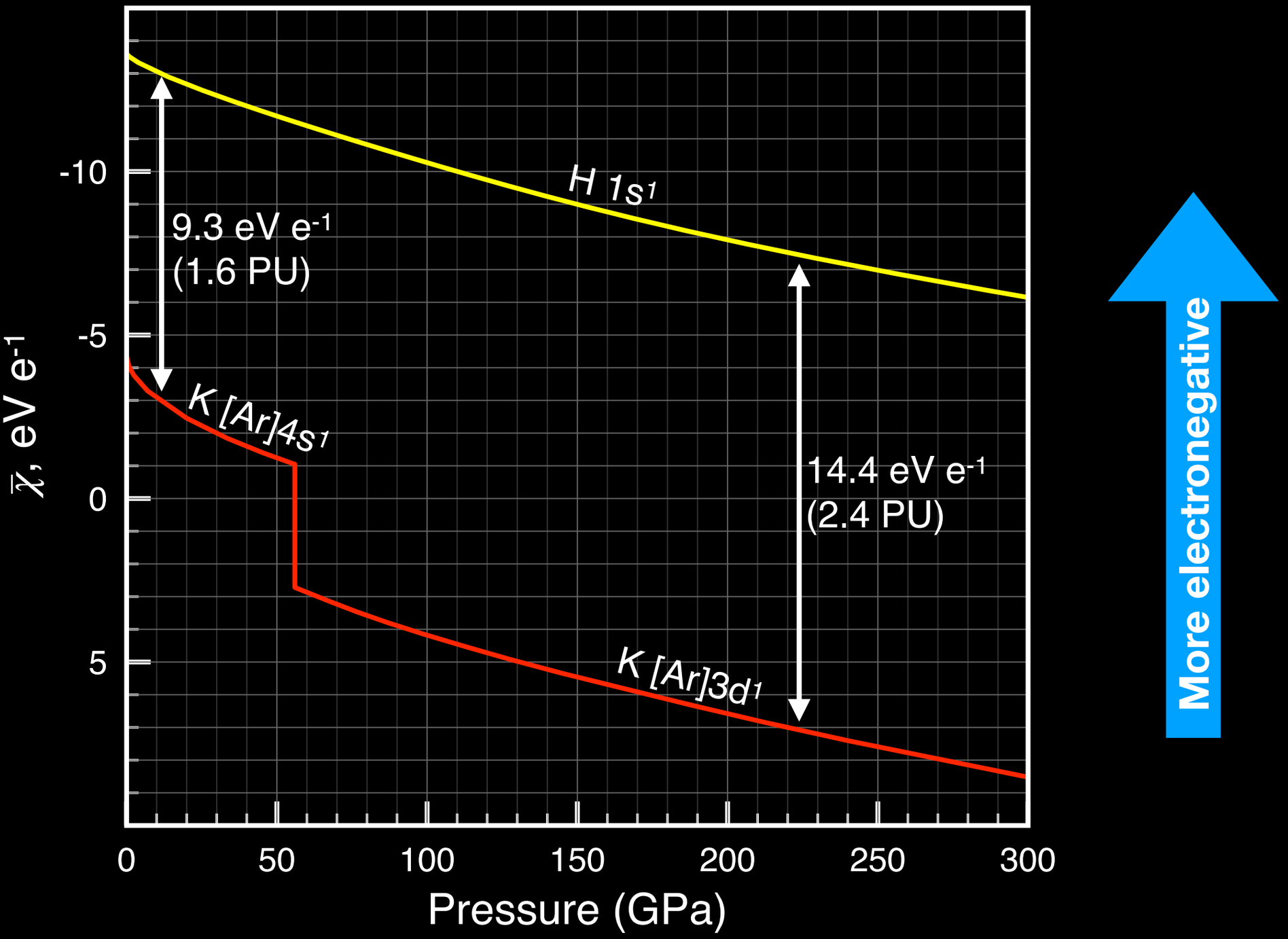
Ground State Electron Configuration



Rahm, M., Cammi, R., N. W. Ashcroft, R. Hoffmann, J. Am. Chem. Soc., 141, 10253-10271, 2019

Changes in Ground State Electron Configuration!



Sternheimer, R. M., *Phys. Rev*, 78, 235-243, 1950.

Parker, L. J., Atou, T., Badding, J. V., *Science*, 273, 95-97, 1996

Rahm, M., Cammi, R., N. W. Ashcroft, R. Hoffmann, *J. Am. Chem. Soc.*, 141, 10253-10271, 2019

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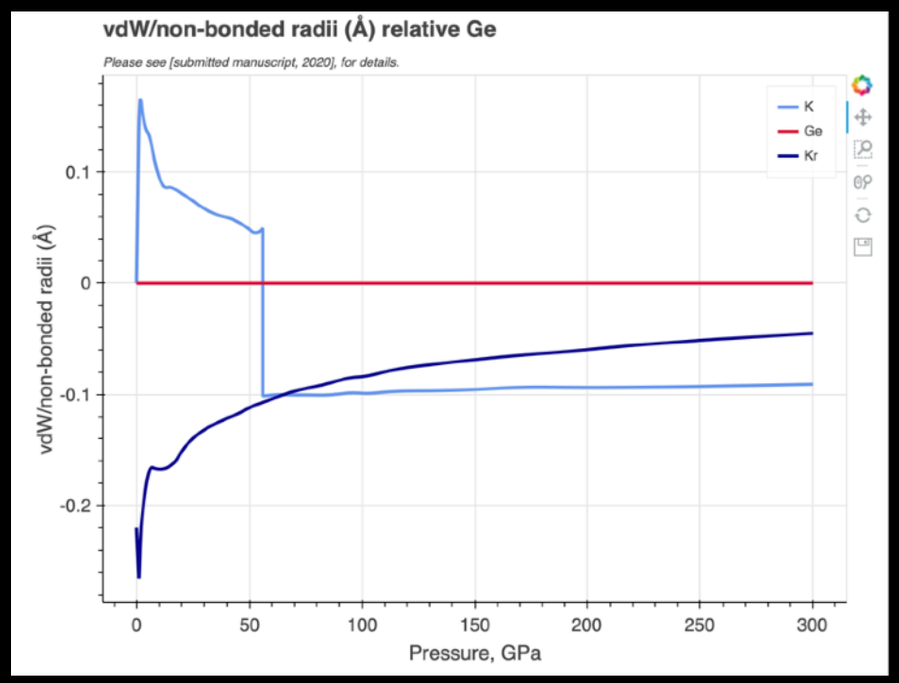
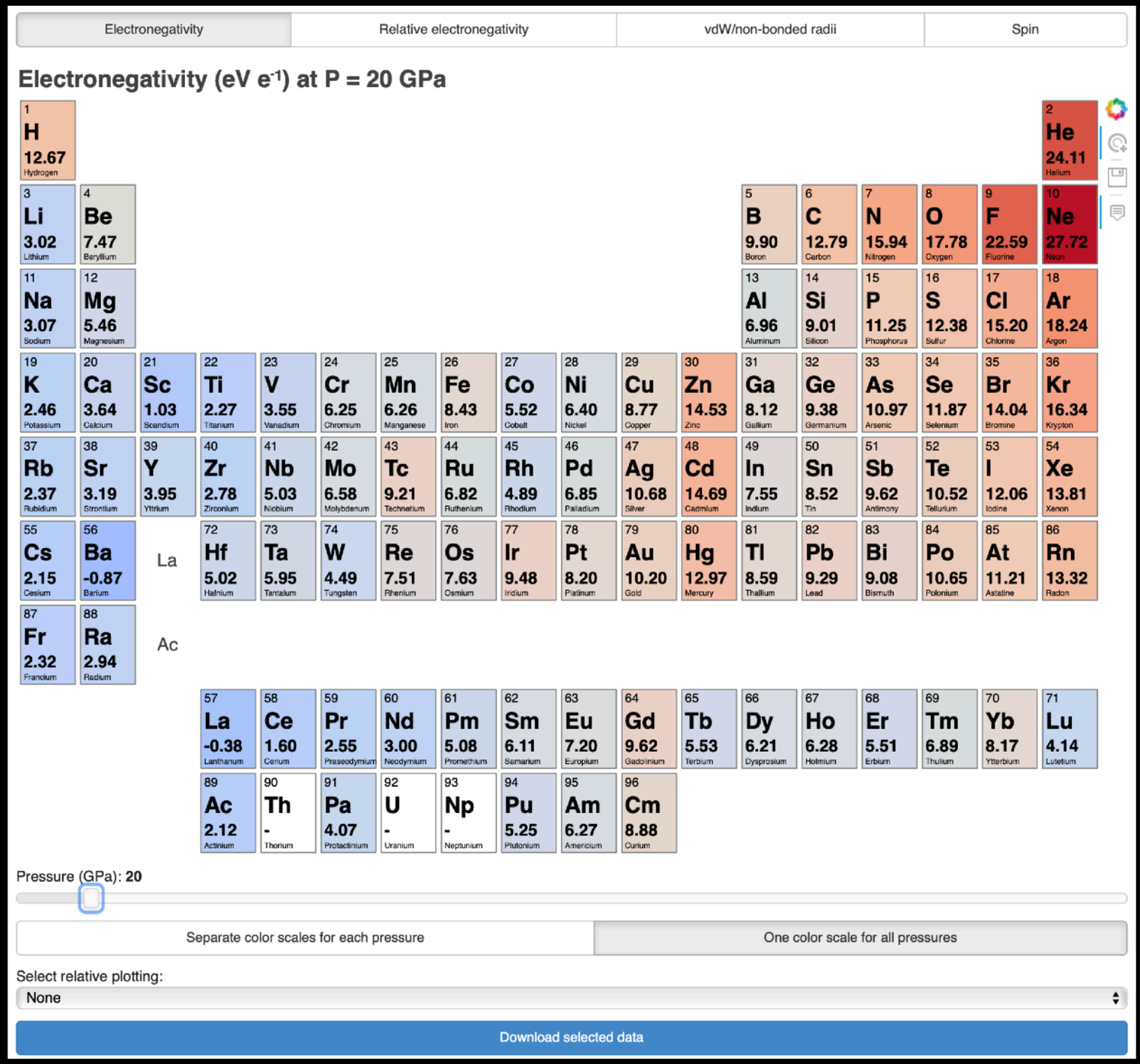
The Atoms Under Pressure Database

https://rahmlab.com/atoms-under-pressure/

- radii
- electronegativity
- electron configuration
- spin

Between 0 to 300 GPa!





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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H 1s^1 *6.1*																	He 1s^2 *20.8*
2	Li 2p^1 *-7.6*	Be 2s^2 *-1.3*											B 2s^{2}2p^1 *2.2*	C 2s^{2}2p^2 *6.6*	N 2s^{2}2p^3 *10.8*	O 2s^{2}2p^4 *13.4*	F 2s^{2}2p^5 *18.7*	Ne 2s^{2}2p^6 *24.4*
3	Na 3s^1 *-3.3*	Mg 3s^2 *-2.3*											Al 3s^{2}3p^1 *-1.6*	Si 3s^{2}3p^2 *0.6*	P 3s^{2}3p^3 *3.8*	S 3s^{2}3p^4 *5.8*	Cl 3s^{2}3p^5 *9.3*	Ar 3s^{2}3p^6 *13.3*
4	K 3d^1 *-8.5*	Ca 3d^2 *-11.5*	Sc 3d^3 *-14.0*	Ti 3d^4 *-12.5*	V 3d^5 *-10.4*	Cr 3d^6 *-7.5*	Mn 3d^7 *-7.7*	Fe 3d^8 *-9.5*	Co 3d^9 *-7.5*	Ni 3d^{10} *-7.1*	Cu 4s^{1}3d^{10} *2.7*	Zn 4s^{2}3d^{10} *8.7*	Ga 4s^{2}4p^1 *1.5*	Ge 4s^{2}4p^2 *2.5*	As 4s^{2}4p^3 *4.1*	Se 4s^{2}4p^4 *5.3*	Br 4s^{2}4p^5 *7.9*	Kr 4s^{2}4p^6 *10.8*
5	Rb 4d^1 *-6.9*	Sr 4d^2 *-10.1*	Y 4d^3 *-10.8*	Zr 4d^4 *-9.8*	Nb 4d^5 *-7.0*	Mo 4d^6 *-5.3*	Tc 4d^7 *-6.7*	Ru 4d^8 *-5.6*	Rh 4d^9 *-4.8*	Pd 4d^{10} *-0.6*	Ag 5s^{1}4d^{10} *4.5*	Cd 5s^{2}4d^{10} *8.8*	In 5s^{2}5p^1 *1.4*	Sn 5s^{2}5p^2 *2.0*	Sb 5s^{2}5p^3 *3.0*	Te 5s^{2}5p^4 *3.9*	I 5s^{2}5p^5 *5.8*	Xe 5s^{2}5p^6 *8.0*
6	Cs 5d^1 *-6.4*	Ba 5d^2 *-9.2*	Lu 5d^3 *-6.4*	Hf 5d^4 *-7.9*	Ta 5d^5 *-7.4*	W 6s^{1}5d^5 *-3.1*	Re 5d^7 *-5.1*	Os 5d^8 *-2.5*	Ir 5d^9 *-3.1*	Pt 5d^{10} *-1.5*	Au 6s^{1}5d^{10} *3.7*	Hg 6s^{2}5d^{10} *7.5*	Tl 6s^{2}6p^1 *2.6*	Pb 6s^{2}6p^2 *3.1*	Bi 6s^{2}6p^3 *2.7*	Po 6s^{2}6p^4 *4.1*	At 6s^{2}6p^5 *4.9*	Rn 6s^{2}6p^6 *7.3*
7	Fr 6d^1 *-5.3*	Ra 6d^2 *-6.4*																

	3	4	5	6	7	8	9	10	11	12
6	La 5d^3 *-9.8*	Ce 5d^{2}4f^2 *-11.7*	Pr 5d^{2}4f^3 *-7.2*	Nd 5d^{2}4f^4 *-7.2*	Pm 5d^{2}4f^5 *-6.8*	Sm 5d^{2}4f^6 *-5.5*	Eu 5d^{2}4f^7 *-4.2*	Gd 5d^{3}4f^7 *0.8*	Tb 5d^{3}4f^8 *1.3*	Dy 5d^{2}4f^{10} *-5.0*
7	Ac 6d^3 *-8.0*		Pa 6d^{3}5f^2 *-10.8*			Pu 6d^{1}5f^7 *-9.2*	Am 6d^{2}5f^7 *-4.1*	Cm 6d^{2}5f^8 *-5.5*		

	13	14	15	16	17
6	Ho 5d^{3}4f^{10} *0.8*	Er 5d^{2}4f^{12} *-5.8*	Tm 5d^{2}4f^{13} *-4.8*	Yb 5d^{2}4f^{14} *-2.1*	

Element
ground state
atom configuration
@ 300 GPa
$\bar{\chi}$

- The electronegativity of Alkali metals are scrambled.
- K is the most electropositive atom in group 1.

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ ***6.1***																	He $1s^2$ ***20.8***
2	Li $2p^1$ ***-7.6***	Be $2s^2$ ***-1.3***											B $2s^22p^1$ ***2.2***	C $2s^22p^2$ ***6.6***	N $2s^22p^3$ ***10.8***	O $2s^22p^4$ ***13.4***	F $2s^22p^5$ ***18.7***	Ne $2s^22p^6$ ***24.4***
3	Na $3s^1$ ***-3.3***	Mg $3s^2$ ***-2.3***											Al $3s^23p^1$ ***-1.6***	Si $3s^23p^2$ ***0.6***	P $3s^23p^3$ ***3.8***	S $3s^23p^4$ ***5.8***	Cl $3s^23p^5$ ***9.3***	Ar $3s^23p^6$ ***13.3***
4	K $3d^1$ ***-8.5***	Ca $3d^2$ ***-11.5***	Sc $3d^3$ ***-14.0***	Ti $3d^4$ ***-12.5***	V $3d^5$ ***-10.4***	Cr $3d^6$ ***-7.5***	Mn $3d^7$ ***-7.7***	Fe $3d^8$ ***-9.5***	Co $3d^9$ ***-7.5***	Ni $3d^{10}$ ***-7.1***	Cu $4s^13d^{10}$ ***2.7***	Zn $4s^23d^{10}$ ***8.7***	Ga $4s^24p^1$ ***1.5***	Ge $4s^24p^2$ ***2.5***	As $4s^24p^3$ ***4.1***	Se $4s^24p^4$ ***5.3***	Br $4s^24p^5$ ***7.9***	Kr $4s^24p^6$ ***10.8***
5	Rb $4d^1$ ***-6.9***	Sr $4d^2$ ***-10.1***	Y $4d^3$ ***-10.8***	Zr $4d^4$ ***-9.8***	Nb $4d^5$ ***-7.0***	Mo $4d^6$ ***-5.3***	Tc $4d^7$ ***-6.7***	Ru $4d^8$ ***-5.6***	Rh $4d^9$ ***-4.8***	Pd $4d^{10}$ ***-0.6***	Ag $5s^14d^{10}$ ***4.5***	Cd $5s^24d^{10}$ ***8.8***	In $5s^25p^1$ ***1.4***	Sn $5s^25p^2$ ***2.0***	Sb $5s^25p^3$ ***3.0***	Te $5s^25p^4$ ***3.9***	I $5s^25p^5$ ***5.8***	Xe $5s^25p^6$ ***8.0***
6	Cs $5d^1$ ***-6.4***	Ba $5d^2$ ***-9.2***	Lu $5d^3$ ***-6.4***	Hf $5d^4$ ***-7.9***	Ta $5d^5$ ***-7.4***	W $6s^15d^5$ ***-3.1***	Re $5d^7$ ***-5.1***	Os $5d^8$ ***-2.5***	Ir $5d^9$ ***-3.1***	Pt $5d^{10}$ ***-1.5***	Au $6s^15d^{10}$ ***3.7***	Hg $6s^25d^{10}$ ***7.5***	Tl $6s^26p^1$ ***2.6***	Pb $6s^26p^2$ ***3.1***	Bi $6s^26p^3$ ***2.7***	Po $6s^26p^4$ ***4.1***	At $6s^26p^5$ ***4.9***	Rn $6s^26p^6$ ***7.3***
7	Fr $6d^1$ ***-5.3***	Ra $6d^2$ ***-6.4***																

	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
6	La $5d^3$ ***-9.8***	Ce $5d^24f^2$ ***-11.7***	Pr $5d^24f^3$ ***-7.2***	Nd $5d^24f^4$ ***-7.2***	Pm $5d^24f^5$ ***-6.8***	Sm $5d^24f^6$ ***-5.5***	Eu $5d^24f^7$ ***-4.2***	Gd $5d^34f^7$ ***0.8***	Tb $5d^34f^8$ ***1.3***	Dy $5d^24f^{10}$ ***-5.0***	Ho $5d^34f^{10}$ ***0.8***	Er $5d^24f^{12}$ ***-5.8***	Tm $5d^24f^{13}$ ***-4.8***	Yb $5d^24f^{14}$ ***-2.1***	
7	Ac $6d^3$ ***-8.0***		Pa $6d^35f^2$ ***-10.8***			Pu $6d^15f^7$ ***-9.2***	Am $6d^25f^7$ ***-4.1***	Cm $6d^25f^8$ ***-5.5***							

Element
ground state atom configuration @ 300 GPa
$\bar{\chi}$

- The electronegativity of the Alkaline earth metals are also scrambled.
- Ca is the most electropositive atom in group 2.

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ *6.1*																	He $1s^2$ *20.8*
2	Li $2p^1$ *-7.6*	Be $2s^2$ *-1.3*											B $2s^22p^1$ *2.2*	C $2s^22p^2$ *6.6*	N $2s^22p^3$ *10.8*	O $2s^22p^4$ *13.4*	F $2s^22p^5$ *18.7*	Ne $2s^22p^6$ *24.4*
3	Na $3s^1$ *-3.3*	Mg $3s^2$ *-2.3*											Al $3s^23p^1$ *-1.6*	Si $3s^23p^2$ *0.6*	P $3s^23p^3$ *3.8*	S $3s^23p^4$ *5.8*	Cl $3s^23p^5$ *9.3*	Ar $3s^23p^6$ *13.3*
4	K $3d^1$ *-8.5*	Ca $3d^2$ *-11.5*	Sc $3d^3$ *-14.0*	Ti $3d^4$ *-12.5*	V $3d^5$ *-10.4*	Cr $3d^6$ *-7.5*	Mn $3d^7$ *-7.7*	Fe $3d^8$ *-9.5*	Co $3d^9$ *-7.5*	Ni $3d^{10}$ *-7.1*	Cu $4s^13d^{10}$ *2.7*	Zn $4s^23d^{10}$ *8.7*	Ga $4s^24p^1$ *1.5*	Ge $4s^24p^2$ *2.5*	As $4s^24p^3$ *4.1*	Se $4s^24p^4$ *5.3*	Br $4s^24p^5$ *7.9*	Kr $4s^24p^6$ *10.8*
5	Rb $4d^1$ *-6.9*	Sr $4d^2$ *-10.1*	Y $4d^3$ *-10.8*	Zr $4d^4$ *-9.8*	Nb $4d^5$ *-7.0*	Mo $4d^6$ *-5.3*	Tc $4d^7$ *-6.7*	Ru $4d^8$ *-5.6*	Rh $4d^9$ *-4.8*	Pd $4d^{10}$ *-0.6*	Ag $5s^14d^{10}$ *4.5*	Cd $5s^24d^{10}$ *8.8*	In $5s^25p^1$ *1.4*	Sn $5s^25p^2$ *2.0*	Sb $5s^25p^3$ *3.0*	Te $5s^25p^4$ *3.9*	I $5s^25p^5$ *5.8*	Xe $5s^25p^6$ *8.0*
6	Cs $5d^1$ *-6.4*	Ba $5d^2$ *-9.2*	Lu $5d^3$ *-6.4*	Hf $5d^4$ *-7.9*	Ta $5d^5$ *-7.4*	W $6s^15d^5$ *-3.1*	Re $5d^7$ *-5.1*	Os $5d^8$ *-2.5*	Ir $5d^9$ *-3.1*	Pt $5d^{10}$ *-1.5*	Au $6s^15d^{10}$ *3.7*	Hg $6s^25d^{10}$ *7.5*	Tl $6s^26p^1$ *2.6*	Pb $6s^26p^2$ *3.1*	Bi $6s^26p^3$ *2.7*	Po $6s^26p^4$ *4.1*	At $6s^26p^5$ *4.9*	Rn $6s^26p^6$ *7.3*
7	Fr $6d^1$ *-5.3*	Ra $6d^2$ *-6.4*																

	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
6	La $5d^3$ *-9.8*	Ce $5d^24f^2$ *-11.7*	Pr $5d^24f^3$ *-7.2*	Nd $5d^24f^4$ *-7.2*	Pm $5d^24f^5$ *-6.8*	Sm $5d^24f^6$ *-5.5*	Eu $5d^24f^7$ *-4.2*	Gd $5d^34f^7$ *0.8*	Tb $5d^34f^8$ *1.3*	Dy $5d^24f^{10}$ *-5.0*	Ho $5d^34f^{10}$ *0.8*	Er $5d^24f^{12}$ *-5.8*	Tm $5d^24f^{13}$ *-4.8*	Yb $5d^24f^{14}$ *-2.1*	
7	Ac $6d^3$ *-8.0*		Pa $6d^35f^2$ *-10.8*			Pu $6d^15f^7$ *-9.2*	Am $6d^25f^7$ *-4.1*	Cm $6d^25f^8$ *-5.5*							

Element
ground state atom configuration @ 300 GPa
$\bar{\chi}$

- several atoms in groups 1 and 2 belong to the transition metal group

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ ***6.1***																	He $1s^2$ ***20.8***
2	Li $2p^1$ ***-7.6***	Be $2s^2$ ***-1.3***											B $2s^22p^1$ ***2.2***	C $2s^22p^2$ ***6.6***	N $2s^22p^3$ ***10.8***	O $2s^22p^4$ ***13.4***	F $2s^22p^5$ ***18.7***	Ne $2s^22p^6$ ***24.4***
3	Na $3s^1$ ***-3.3***	Mg $3s^2$ ***-2.3***											Al $3s^23p^1$ ***-1.6***	Si $3s^23p^2$ ***0.6***	P $3s^23p^3$ ***3.8***	S $3s^23p^4$ ***5.8***	Cl $3s^23p^5$ ***9.3***	Ar $3s^23p^6$ ***13.3***
4	K $3d^1$ ***-8.5***	Ca $3d^2$ ***-11.5***	Sc $3d^3$ ***-14.0***	Ti $3d^4$ ***-12.5***	V $3d^5$ ***-10.4***	Cr $3d^6$ ***-7.5***	Mn $3d^7$ ***-7.7***	Fe $3d^8$ ***-9.5***	Co $3d^9$ ***-7.5***	Ni $3d^{10}$ ***-7.1***	Cu $4s^13d^{10}$ ***2.7***	Zn $4s^23d^{10}$ ***8.7***	Ga $4s^24p^1$ ***1.5***	Ge $4s^24p^2$ ***2.5***	As $4s^24p^3$ ***4.1***	Se $4s^24p^4$ ***5.3***	Br $4s^24p^5$ ***7.9***	Kr $4s^24p^6$ ***10.8***
5	Rb $4d^1$ ***-6.9***	Sr $4d^2$ ***-10.1***	Y $4d^3$ ***-10.8***	Zr $4d^4$ ***-9.8***	Nb $4d^5$ ***-7.0***	Mo $4d^6$ ***-5.3***	Tc $4d^7$ ***-6.7***	Ru $4d^8$ ***-5.6***	Rh $4d^9$ ***-4.8***	Pd $4d^{10}$ ***-0.6***	Ag $5s^14d^{10}$ ***4.5***	Cd $5s^24d^{10}$ ***8.8***	In $5s^25p^1$ ***1.4***	Sn $5s^25p^2$ ***2.0***	Sb $5s^25p^3$ ***3.0***	Te $5s^25p^4$ ***3.9***	I $5s^25p^5$ ***5.8***	Xe $5s^25p^6$ ***8.0***
6	Cs $5d^1$ ***-6.4***	Ba $5d^2$ ***-9.2***	Lu $5d^3$ ***-6.4***	Hf $5d^4$ ***-7.9***	Ta $5d^5$ ***-7.4***	W $6s^15d^5$ ***-3.1***	Re $5d^7$ ***-5.1***	Os $5d^8$ ***-2.5***	Ir $5d^9$ ***-3.1***	Pt $5d^{10}$ ***-1.5***	Au $6s^15d^{10}$ ***3.7***	Hg $6s^25d^{10}$ ***7.5***	Tl $6s^26p^1$ ***2.6***	Pb $6s^26p^2$ ***3.1***	Bi $6s^26p^3$ ***2.7***	Po $6s^26p^4$ ***4.1***	At $6s^26p^5$ ***4.9***	Rn $6s^26p^6$ ***7.3***
7	Fr $6d^1$ ***-5.3***	Ra $6d^2$ ***-6.4***																
6			La $5d^3$ ***-9.8***	Ce $5d^24f^2$ ***-11.7***	Pr $5d^24f^3$ ***-7.2***	Nd $5d^24f^4$ ***-7.2***	Pm $5d^24f^5$ ***-6.8***	Sm $5d^24f^6$ ***-5.5***	Eu $5d^24f^7$ ***-4.2***	Gd $5d^34f^7$ ***0.8***	Tb $5d^34f^8$ ***1.3***	Dy $5d^24f^{10}$ ***-5.0***	Ho $5d^34f^{10}$ ***0.8***	Er $5d^24f^{12}$ ***-5.8***	Tm $5d^24f^{13}$ ***-4.8***	Yb $5d^24f^{14}$ ***-2.1***	**Element** ground state atom configuration @ 300 GPa $\overline{\chi}$
7			Ac $6d^3$ ***-8.0***		Pa $6d^35f^2$ ***-10.8***			Pu $6d^15f^7$ ***-9.2***	Am $6d^25f^7$ ***-4.1***	Cm $6d^25f^8$ ***-5.5***								

- The *Aufbau* principle is strengthened under pressure
- Hund's rule is never violated in the investigated pressure range

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ ***6.1***																	He $1s^2$ ***20.8***
2	Li $2p^1$ ***-7.6***	Be $2s^2$ ***-1.3***											B $2s^22p^1$ ***2.2***	C $2s^22p^2$ ***6.6***	N $2s^22p^3$ ***10.8***	O $2s^22p^4$ ***13.4***	F $2s^22p^5$ ***18.7***	Ne $2s^22p^6$ ***24.4***
3	Na $3s^1$ ***-3.3***	Mg $3s^2$ ***-2.3***											Al $3s^23p^1$ ***-1.6***	Si $3s^23p^2$ ***0.6***	P $3s^23p^3$ ***3.8***	S $3s^23p^4$ ***5.8***	Cl $3s^23p^5$ ***9.3***	Ar $3s^23p^6$ ***13.3***
4	K $3d^1$ ***-8.5***	Ca $3d^2$ ***-11.5***	Sc $3d^3$ ***-14.0***	Ti $3d^4$ ***-12.5***	V $3d^5$ ***-10.4***	Cr $3d^6$ ***-7.5***	Mn $3d^7$ ***-7.7***	Fe $3d^8$ ***-9.5***	Co $3d^9$ ***-7.5***	Ni $3d^{10}$ ***-7.1***	Cu $4s^13d^{10}$ ***2.7***	Zn $4s^23d^{10}$ ***8.7***	Ga $4s^24p^1$ ***1.5***	Ge $4s^24p^2$ ***2.5***	As $4s^24p^3$ ***4.1***	Se $4s^24p^4$ ***5.3***	Br $4s^24p^5$ ***7.9***	Kr $4s^24p^6$ ***10.8***
5	Rb $4d^1$ ***-6.9***	Sr $4d^2$ ***-10.1***	Y $4d^3$ ***-10.8***	Zr $4d^4$ ***-9.8***	Nb $4d^5$ ***-7.0***	Mo $4d^6$ ***-5.3***	Tc $4d^7$ ***-6.7***	Ru $4d^8$ ***-5.6***	Rh $4d^9$ ***-4.8***	Pd $4d^{10}$ ***-0.6***	Ag $5s^14d^{10}$ ***4.5***	Cd $5s^24d^{10}$ ***8.8***	In $5s^25p^1$ ***1.4***	Sn $5s^25p^2$ ***2.0***	Sb $5s^25p^3$ ***3.0***	Te $5s^25p^4$ ***3.9***	I $5s^25p^5$ ***5.8***	Xe $5s^25p^6$ ***8.0***
6	Cs $5d^1$ ***-6.4***	Ba $5d^2$ ***-9.2***	Lu $5d^3$ ***-6.4***	Hf $5d^4$ ***-7.9***	Ta $5d^5$ ***-7.4***	W $6s^15d^5$ ***-3.1***	Re $5d^7$ ***-5.1***	Os $5d^8$ ***-2.5***	Ir $5d^9$ ***-3.1***	Pt $5d^{10}$ ***-1.5***	Au $6s^15d^{10}$ ***3.7***	Hg $6s^25d^{10}$ ***7.5***	Tl $6s^26p^1$ ***2.6***	Pb $6s^26p^2$ ***3.1***	Bi $6s^26p^3$ ***2.7***	Po $6s^26p^4$ ***4.1***	At $6s^26p^5$ ***4.9***	Rn $6s^26p^6$ ***7.3***
7	Fr $6d^1$ ***-5.3***	Ra $6d^2$ ***-6.4***																
6			La $5d^3$ ***-9.8***	Ce $5d^24f^2$ ***-11.7***	Pr $5d^24f^3$ ***-7.2***	Nd $5d^24f^4$ ***-7.2***	Pm $5d^24f^5$ ***-6.8***	Sm $5d^24f^6$ ***-5.5***	Eu $5d^24f^7$ ***-4.2***	Gd $5d^34f^7$ ***0.8***	Tb $5d^34f^8$ ***1.3***	Dy $5d^24f^{10}$ ***-5.0***	Ho $5d^34f^{10}$ ***0.8***	Er $5d^24f^{12}$ ***-5.8***	Tm $5d^24f^{13}$ ***-4.8***	Yb $5d^24f^{14}$ ***-2.1***	**Element** ground state atom configuration @ 300 GPa $\overline{\chi}$
7			Ac $6d^3$ ***-8.0***		Pa $6d^35f^2$ ***-10.8***			Pu $6d^15f^7$ ***-9.2***	Am $6d^25f^7$ ***-4.1***	Cm $6d^25f^8$ ***-5.5***								

- Lithium becomes a p-block element

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ *6.1*																	He $1s^2$ *20.8*
2	Li $2p^1$ *-7.6*	Be $2s^2$ *-1.3*											B $2s^22p^1$ *2.2*	C $2s^22p^2$ *6.6*	N $2s^22p^3$ *10.8*	O $2s^22p^4$ *13.4*	F $2s^22p^5$ *18.7*	Ne $2s^22p^6$ *24.4*
3	Na $3s^1$ *-3.3*	Mg $3s^2$ *-2.3*											Al $3s^23p^1$ *-1.6*	Si $3s^23p^2$ *0.6*	P $3s^23p^3$ *3.8*	S $3s^23p^4$ *5.8*	Cl $3s^23p^5$ *9.3*	Ar $3s^23p^6$ *13.3*
4	K $3d^1$ *-8.5*	Ca $3d^2$ *-11.5*	Sc $3d^3$ *-14.0*	Ti $3d^4$ *-12.5*	V $3d^5$ *-10.4*	Cr $3d^6$ *-7.5*	Mn $3d^7$ *-7.7*	Fe $3d^8$ *-9.5*	Co $3d^9$ *-7.5*	Ni $3d^{10}$ *-7.1*	Cu $4s^13d^{10}$ *2.7*	Zn $4s^23d^{10}$ *8.7*	Ga $4s^24p^1$ *1.5*	Ge $4s^24p^2$ *2.5*	As $4s^24p^3$ *4.1*	Se $4s^24p^4$ *5.3*	Br $4s^24p^5$ *7.9*	Kr $4s^24p^6$ *10.8*
5	Rb $4d^1$ *-6.9*	Sr $4d^2$ *-10.1*	Y $4d^3$ *-10.8*	Zr $4d^4$ *-9.8*	Nb $4d^5$ *-7.0*	Mo $4d^6$ *-5.3*	Tc $4d^7$ *-6.7*	Ru $4d^8$ *-5.6*	Rh $4d^9$ *-4.8*	Pd $4d^{10}$ *-0.6*	Ag $5s^14d^{10}$ *4.5*	Cd $5s^24d^{10}$ *8.8*	In $5s^25p^1$ *1.4*	Sn $5s^25p^2$ *2.0*	Sb $5s^25p^3$ *3.0*	Te $5s^25p^4$ *3.9*	I $5s^25p^5$ *5.8*	Xe $5s^25p^6$ *8.0*
6	Cs $5d^1$ *-6.4*	Ba $5d^2$ *-9.2*	Lu $5d^3$ *-6.4*	Hf $5d^4$ *-7.9*	Ta $5d^5$ *-7.4*	W $6s^15d^5$ *-3.1*	Re $5d^7$ *-5.1*	Os $5d^8$ *-2.5*	Ir $5d^9$ *-3.1*	Pt $5d^{10}$ *-1.5*	Au $6s^15d^{10}$ *3.7*	Hg $6s^25d^{10}$ *7.5*	Tl $6s^26p^1$ *2.6*	Pb $6s^26p^2$ *3.1*	Bi $6s^26p^3$ *2.7*	Po $6s^26p^4$ *4.1*	At $6s^26p^5$ *4.9*	Rn $6s^26p^6$ *7.3*
7	Fr $6d^1$ *-5.3*	Ra $6d^2$ *-6.4*																
6			La $5d^3$ *-9.8*	Ce $5d^24f^2$ *-11.7*	Pr $5d^24f^3$ *-7.2*	Nd $5d^24f^4$ *-7.2*	Pm $5d^24f^5$ *-6.8*	Sm $5d^24f^6$ *-5.5*	Eu $5d^24f^7$ *-4.2*	Gd $5d^34f^7$ *0.8*	Tb $5d^34f^8$ *1.3*	Dy $5d^24f^{10}$ *-5.0*	Ho $5d^34f^{10}$ *0.8*	Er $5d^24f^{12}$ *-5.8*	Tm $5d^24f^{13}$ *-4.8*	Yb $5d^24f^{14}$ *-2.1*	**Element** ground state atom configuration @ 300 GPa $\bar{\chi}$
7			Ac $6d^3$ *-8.0*		Pa $6d^35f^2$ *-10.8*			Pu $6d^15f^7$ *-9.2*	Am $6d^25f^7$ *-4.1*	Cm $6d^25f^8$ *-5.5*								

- Atoms in group 10 all takes on the same valence configuration.

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ ***6.1***																	He $1s^2$ ***20.8***
2	Li $2p^1$ ***-7.6***	Be $2s^2$ ***-1.3***											B $2s^22p^1$ ***2.2***	C $2s^22p^2$ ***6.6***	N $2s^22p^3$ ***10.8***	O $2s^22p^4$ ***13.4***	F $2s^22p^5$ ***18.7***	Ne $2s^22p^6$ ***24.4***
3	Na $3s^1$ ***-3.3***	Mg $3s^2$ ***-2.3***											Al $3s^23p^1$ ***-1.6***	Si $3s^23p^2$ ***0.6***	P $3s^23p^3$ ***3.8***	S $3s^23p^4$ ***5.8***	Cl $3s^23p^5$ ***9.3***	Ar $3s^23p^6$ ***13.3***
4	K $3d^1$ ***-8.5***	Ca $3d^2$ ***-11.5***	Sc $3d^3$ ***-14.0***	Ti $3d^4$ ***-12.5***	V $3d^5$ ***-10.4***	Cr $3d^6$ ***-7.5***	Mn $3d^7$ ***-7.7***	Fe $3d^8$ ***-9.5***	Co $3d^9$ ***-7.5***	Ni $3d^{10}$ ***-7.1***	Cu $4s^13d^{10}$ ***2.7***	Zn $4s^23d^{10}$ ***8.7***	Ga $4s^24p^1$ ***1.5***	Ge $4s^24p^2$ ***2.5***	As $4s^24p^3$ ***4.1***	Se $4s^24p^4$ ***5.3***	Br $4s^24p^5$ ***7.9***	Kr $4s^24p^6$ ***10.8***
5	Rb $4d^1$ ***-6.9***	Sr $4d^2$ ***-10.1***	Y $4d^3$ ***-10.8***	Zr $4d^4$ ***-9.8***	Nb $4d^5$ ***-7.0***	Mo $4d^6$ ***-5.3***	Tc $4d^7$ ***-6.7***	Ru $4d^8$ ***-5.6***	Rh $4d^9$ ***-4.8***	Pd $4d^{10}$ ***-0.6***	Ag $5s^14d^{10}$ ***4.5***	Cd $5s^24d^{10}$ ***8.8***	In $5s^25p^1$ ***1.4***	Sn $5s^25p^2$ ***2.0***	Sb $5s^25p^3$ ***3.0***	Te $5s^25p^4$ ***3.9***	I $5s^25p^5$ ***5.8***	Xe $5s^25p^6$ ***8.0***
6	Cs $5d^1$ ***-6.4***	Ba $5d^2$ ***-9.2***	Lu $5d^3$ ***-6.4***	Hf $5d^4$ ***-7.9***	Ta $5d^5$ ***-7.4***	W $6s^15d^5$ ***-3.1***	Re $5d^7$ ***-5.1***	Os $5d^8$ ***-2.5***	Ir $5d^9$ ***-3.1***	Pt $5d^{10}$ ***-1.5***	Au $6s^15d^{10}$ ***3.7***	Hg $6s^25d^{10}$ ***7.5***	Tl $6s^26p^1$ ***2.6***	Pb $6s^26p^2$ ***3.1***	Bi $6s^26p^3$ ***2.7***	Po $6s^26p^4$ ***4.1***	At $6s^26p^5$ ***4.9***	Rn $6s^26p^6$ ***7.3***
7	Fr $6d^1$ ***-5.3***	Ra $6d^2$ ***-6.4***																
6			La $5d^3$ ***-9.8***	Ce $5d^24f^2$ ***-11.7***	Pr $5d^24f^3$ ***-7.2***	Nd $5d^24f^4$ ***-7.2***	Pm $5d^24f^5$ ***-6.8***	Sm $5d^24f^6$ ***-5.5***	Eu $5d^24f^7$ ***-4.2***	Gd $5d^34f^7$ ***0.8***	Tb $5d^34f^8$ ***1.3***	Dy $5d^24f^{10}$ ***-5.0***	Ho $5d^34f^{10}$ ***0.8***	Er $5d^24f^{12}$ ***-5.8***	Tm $5d^24f^{13}$ ***-4.8***	Yb $5d^24f^{14}$ ***-2.1***	
7			Ac $6d^3$ ***-8.0***		Pa $6d^35f^2$ ***-10.8***			Pu $6d^15f^7$ ***-9.2***	Am $6d^25f^7$ ***-4.1***	Cm $6d^25f^8$ ***-5.5***								

Element
ground state atom configuration @ 300 GPa
$\overline{\chi}$

- Chemical differences in the f-block are significantly amplified.

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ ***6.1***																	He $1s^2$ ***20.8***
2	Li $2p^1$ ***-7.6***	Be $2s^2$ ***-1.3***											B $2s^22p^1$ ***2.2***	C $2s^22p^2$ ***6.6***	N $2s^22p^3$ ***10.8***	O $2s^22p^4$ ***13.4***	F $2s^22p^5$ ***18.7***	Ne $2s^22p^6$ ***24.4***
3	Na $3s^1$ ***-3.3***	Mg $3s^2$ ***-2.3***											Al $3s^23p^1$ ***-1.6***	Si $3s^23p^2$ ***0.6***	P $3s^23p^3$ ***3.8***	S $3s^23p^4$ ***5.8***	Cl $3s^23p^5$ ***9.3***	Ar $3s^23p^6$ ***13.3***
4	K $3d^1$ ***-8.5***	Ca $3d^2$ ***-11.5***	Sc $3d^3$ ***-14.0***	Ti $3d^4$ ***-12.5***	V $3d^5$ ***-10.4***	Cr $3d^6$ ***-7.5***	Mn $3d^7$ ***-7.7***	Fe $3d^8$ ***-9.5***	Co $3d^9$ ***-7.5***	Ni $3d^{10}$ ***-7.1***	Cu $4s^13d^{10}$ ***2.7***	Zn $4s^23d^{10}$ ***8.7***	Ga $4s^24p^1$ ***1.5***	Ge $4s^24p^2$ ***2.5***	As $4s^24p^3$ ***4.1***	Se $4s^24p^4$ ***5.3***	Br $4s^24p^5$ ***7.9***	Kr $4s^24p^6$ ***10.8***
5	Rb $4d^1$ ***-6.9***	Sr $4d^2$ ***-10.1***	Y $4d^3$ ***-10.8***	Zr $4d^4$ ***-9.8***	Nb $4d^5$ ***-7.0***	Mo $4d^6$ ***-5.3***	Tc $4d^7$ ***-6.7***	Ru $4d^8$ ***-5.6***	Rh $4d^9$ ***-4.8***	Pd $4d^{10}$ ***-0.6***	Ag $5s^14d^{10}$ ***4.5***	Cd $5s^24d^{10}$ ***8.8***	In $5s^25p^1$ ***1.4***	Sn $5s^25p^2$ ***2.0***	Sb $5s^25p^3$ ***3.0***	Te $5s^25p^4$ ***3.9***	I $5s^25p^5$ ***5.8***	Xe $5s^25p^6$ ***8.0***
6	Cs $5d^1$ ***-6.4***	Ba $5d^2$ ***-9.2***	Lu $5d^3$ ***-6.4***	Hf $5d^4$ ***-7.9***	Ta $5d^5$ ***-7.4***	W $6s^15d^5$ ***-3.1***	Re $5d^7$ ***-5.1***	Os $5d^8$ ***-2.5***	Ir $5d^9$ ***-3.1***	Pt $5d^{10}$ ***-1.5***	Au $6s^15d^{10}$ ***3.7***	Hg $6s^25d^{10}$ ***7.5***	Tl $6s^26p^1$ ***2.6***	Pb $6s^26p^2$ ***3.1***	Bi $6s^26p^3$ ***2.7***	Po $6s^26p^4$ ***4.1***	At $6s^26p^5$ ***4.9***	Rn $6s^26p^6$ ***7.3***
7	Fr $6d^1$ ***-5.3***	Ra $6d^2$ ***-6.4***																
6			La $5d^3$ ***-9.8***	Ce $5d^24f^2$ ***-11.7***	Pr $5d^24f^3$ ***-7.2***	Nd $5d^24f^4$ ***-7.2***	Pm $5d^24f^5$ ***-6.8***	Sm $5d^24f^6$ ***-5.5***	Eu $5d^24f^7$ ***-4.2***	Gd $5d^34f^7$ ***0.8***	Tb $5d^34f^8$ ***1.3***	Dy $5d^24f^{10}$ ***-5.0***	Ho $5d^34f^{10}$ ***0.8***	Er $5d^24f^{12}$ ***-5.8***	Tm $5d^24f^{13}$ ***-4.8***	Yb $5d^24f^{14}$ ***-2.1***	**Element** ground state atom configuration @ 300 GPa $\overline{\chi}$
7			Ac $6d^3$ ***-8.0***		Pa $6d^35f^2$ ***-10.8***			Pu $6d^15f^7$ ***-9.2***	Am $6d^25f^7$ ***-4.1***	Cm $6d^25f^8$ ***-5.5***								

- Sc is the least electronegative of all atoms.
- Scandium fluoride is the most ionic compound

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ ***6.1***																	He $1s^2$ ***20.8***
2	Li $2p^1$ ***-7.6***	Be $2s^2$ ***-1.3***											B $2s^22p^1$ ***2.2***	C $2s^22p^2$ ***6.6***	N $2s^22p^3$ ***10.8***	O $2s^22p^4$ ***13.4***	F $2s^22p^5$ ***18.7***	Ne $2s^22p^6$ ***24.4***
3	Na $3s^1$ ***-3.3***	Mg $3s^2$ ***-2.3***											Al $3s^23p^1$ ***-1.6***	Si $3s^23p^2$ ***0.6***	P $3s^23p^3$ ***3.8***	S $3s^23p^4$ ***5.8***	Cl $3s^23p^5$ ***9.3***	Ar $3s^23p^6$ ***13.3***
4	K $3d^1$ ***-8.5***	Ca $3d^2$ ***-11.5***	Sc $3d^3$ ***-14.0***	Ti $3d^4$ ***-12.5***	V $3d^5$ ***-10.4***	Cr $3d^6$ ***-7.5***	Mn $3d^7$ ***-7.7***	Fe $3d^8$ ***-9.5***	Co $3d^9$ ***-7.5***	Ni $3d^{10}$ ***-7.1***	Cu $4s^13d^{10}$ ***2.7***	Zn $4s^23d^{10}$ ***8.7***	Ga $4s^24p^1$ ***1.5***	Ge $4s^24p^2$ ***2.5***	As $4s^24p^3$ ***4.1***	Se $4s^24p^4$ ***5.3***	Br $4s^24p^5$ ***7.9***	Kr $4s^24p^6$ ***10.8***
5	Rb $4d^1$ ***-6.9***	Sr $4d^2$ ***-10.1***	Y $4d^3$ ***-10.8***	Zr $4d^4$ ***-9.8***	Nb $4d^5$ ***-7.0***	Mo $4d^6$ ***-5.3***	Tc $4d^7$ ***-6.7***	Ru $4d^8$ ***-5.6***	Rh $4d^9$ ***-4.8***	Pd $4d^{10}$ ***-0.6***	Ag $5s^14d^{10}$ ***4.5***	Cd $5s^24d^{10}$ ***8.8***	In $5s^25p^1$ ***1.4***	Sn $5s^25p^2$ ***2.0***	Sb $5s^25p^3$ ***3.0***	Te $5s^25p^4$ ***3.9***	I $5s^25p^5$ ***5.8***	Xe $5s^25p^6$ ***8.0***
6	Cs $5d^1$ ***-6.4***	Ba $5d^2$ ***-9.2***	Lu $5d^3$ ***-6.4***	Hf $5d^4$ ***-7.9***	Ta $5d^5$ ***-7.4***	W $6s^15d^5$ ***-3.1***	Re $5d^7$ ***-5.1***	Os $5d^8$ ***-2.5***	Ir $5d^9$ ***-3.1***	Pt $5d^{10}$ ***-1.5***	Au $6s^15d^{10}$ ***3.7***	Hg $6s^25d^{10}$ ***7.5***	Tl $6s^26p^1$ ***2.6***	Pb $6s^26p^2$ ***3.1***	Bi $6s^26p^3$ ***2.7***	Po $6s^26p^4$ ***4.1***	At $6s^26p^5$ ***4.9***	Rn $6s^26p^6$ ***7.3***
7	Fr $6d^1$ ***-5.3***	Ra $6d^2$ ***-6.4***																

	3	4	5	6	7	8	9	10	11	12
6	La $5d^3$ ***-9.8***	Ce $5d^24f^2$ ***-11.7***	Pr $5d^24f^3$ ***-7.2***	Nd $5d^24f^4$ ***-7.2***	Pm $5d^24f^5$ ***-6.8***	Sm $5d^24f^6$ ***-5.5***	Eu $5d^24f^7$ ***-4.2***	Gd $5d^34f^7$ ***0.8***	Tb $5d^34f^8$ ***1.3***	Dy $5d^24f^{10}$ ***-5.0***
7	Ac $6d^3$ ***-8.0***		Pa $6d^35f^2$ ***-10.8***			Pu $6d^15f^7$ ***-9.2***	Am $6d^25f^7$ ***-4.1***	Cm $6d^25f^8$ ***-5.5***		

	13	14	15	16	17
6	Ho $5d^34f^{10}$ ***0.8***	Er $5d^24f^{12}$ ***-5.8***	Tm $5d^24f^{13}$ ***-4.8***	Yb $5d^24f^{14}$ ***-2.1***	**Element** ground state atom configuration @ 300 GPa $\overline{\chi}$

- It is “easier” to fluorinate… <u>anything</u> under pressure.

F $2s^22p^5$ ***23.3*** | I $5s^25p^5$ ***13.4*** @1atm

Nature Reviews Chemistry | https://doi.org/10.1038/s41570-019-0072-8 | Published online: 22 January 2019

MAIN-GROUP CHEMISTRY

I will bond IF hard pressed

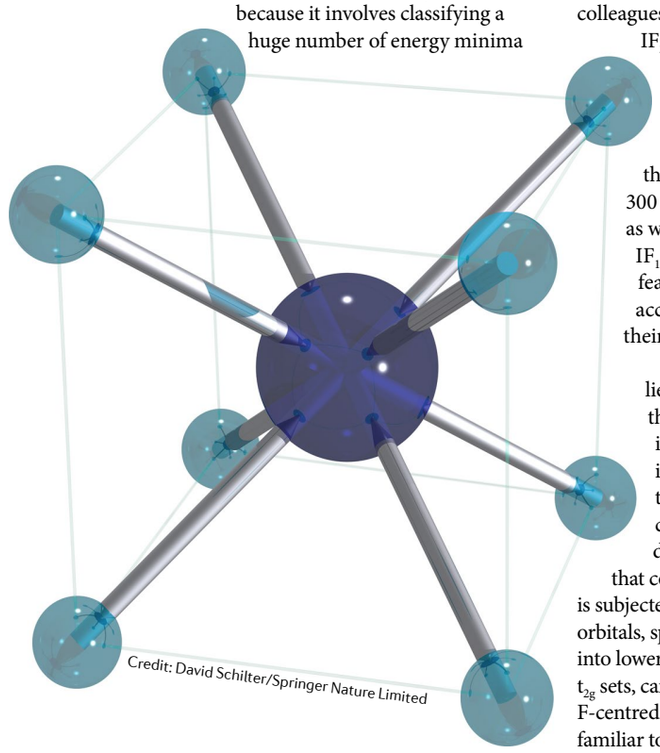
> there is a growing need to expand our chemical design intuition to encompass the high-pressure regime

Being relatively small and electronegative, halogen atoms feature in a great number of high-valent species, such as $NaCl_3$, HgF_4 and IF_7. The latter features heptacoordinate I(VII) — the highest coordination number for a main-group atom in a neutral compound. The chemical space occupied by iodine fluorides is rich, especially when one considers what can form at high pressures. A team led by Guochun Yang, Yan-ming Ma and Martin Rahm have used computational methods to survey this vast space, and they describe in *Chemical Science* how they came across IF_8 as an energetically viable octacoordinate compound.

"Atomistic structure prediction of materials is extremely difficult because it involves classifying a huge number of energy minima on a multidimensional lattice energy surface," reflects Ma. A particularly efficient way to explore such a surface is particle swarm optimization, whereby several potential solutions are each guided towards energy minima according to both the viability of their present positions and the viability of other solution positions. Beginning with I:F ratios, temperature ($T \rightarrow 0$) and pressure as inputs, one can search a surface for minimum energy structures, which can subsequently be optimized using density functional theory.

At ambient pressure, IF_3, IF_5 and IF_7 exist as distorted T-shaped, square-pyramidal and pentagonal-biypyramidal molecules, respectively. When the pressure is ramped up in silico, Yang, Ma, Rahm and colleagues predict, for example, that IF_3 polymerizes (23 GPa) before decomposing into IF_5 and I_2 (140 GPa). The team also discovered new species that are thermodynamically stable at 300 GPa. These include IF_8 as well as the higher fluorides IF_{10}, IF_{11} and IF_{12} that also feature octacoordinate I on account of having 'free' F_2 in their lattices.

In atomic I, the 5d orbitals lie so high in energy above the 5p set that hybridization is impossible. The situation is very different when the same I atom is at the centre of a distorted cube defined by eight F atoms that come close when the system is subjected to 300 GPa. Here, the 5d orbitals, split by the cubic ligand field into lower-lying e_g and higher-lying t_{2g} sets, can overlap with filled F-centred orbitals in an interaction familiar to inorganic chemists.



Credit: David Schilter/Springer Nature Limited

The team computed the relative occupancies of the I-centred valence orbitals to be $s^1p^{1.7}d^1$, confirming the relevance of the 5d set to the frontier molecular orbitals of IF_8, a truly hypervalent molecule. At ambient pressure, the anion $[IF_8]^-$ has a square antiprismatic I(VII) centre and is also hypercoordinated. However, the I 5d orbitals are too high in energy to participate in covalent bonding and it would be contentious to call $[IF_8]^-$ hypervalent.

Yang and co-workers acquired independent evidence for the involvement of 5d orbitals in the bonding of IF_8 by calculating its projected density of (electronic) states, which indicates mixing of I 5d orbitals with other I and F valence orbitals. Moreover, the Fermi level intersects the F 2p band, suggesting that crystalline IF_8 is metallic and has F-centred vacancies. Thus, IF_8 is not an I(VIII) complex but is best considered an I(VII) centre surrounded by a set of eight F^- ligands in which there is one (delocalized) hole.

Although predicted to be stable at high pressures and ultralow temperatures, IF_8 is dynamically unstable towards dissociation under ambient pressure — a likely reason why this compound, which would be challenging to prepare, has escaped the attention of many. Rahm points out "there is a growing need to expand our chemical design intuition to encompass the high-pressure regime." Only then will we see how far we can push hypercoordination and hypervalence in main-group compounds.

David Schilter

ORIGINAL ARTICLE Luo, D. et al. A hypervalent and cubically coordinated molecular phase of IF_8 predicted at high pressure. *Chem. Sci.* https://doi.org/10.1039/C8SC04635B (2019)

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Predictions

Electronegativity of the Atoms

@ 300 GPa (eV e^{-1})

6 eV e^{-1} ≈ 1 Pauling unit

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H $1s^1$ *6.1*																	He $1s^2$ *20.8*
2	Li $2p^1$ *-7.6*	Be $2s^2$ *-1.3*											B $2s^22p^1$ *2.2*	C $2s^22p^2$ *6.6*	N $2s^22p^3$ *10.8*	O $2s^22p^4$ *13.4*	F $2s^22p^5$ *18.7*	Ne $2s^22p^6$ *24.4*
3	Na $3s^1$ *-3.3*	Mg $3s^2$ *-2.3*											Al $3s^23p^1$ *-1.6*	Si $3s^23p^2$ *0.6*	P $3s^23p^3$ *3.8*	S $3s^23p^4$ *5.8*	Cl $3s^23p^5$ *9.3*	Ar $3s^23p^6$ *13.3*
4	K $3d^1$ *-8.5*	Ca $3d^2$ *-11.5*	Sc $3d^3$ *-14.0*	Ti $3d^4$ *-12.5*	V $3d^5$ *-10.4*	Cr $3d^6$ *-7.5*	Mn $3d^7$ *-7.7*	Fe $3d^8$ *-9.5*	Co $3d^9$ *-7.5*	Ni $3d^{10}$ *-7.1*	Cu $4s^13d^{10}$ *2.7*	Zn $4s^23d^{10}$ *8.7*	Ga $4s^24p^1$ *1.5*	Ge $4s^24p^2$ *2.5*	As $4s^24p^3$ *4.1*	Se $4s^24p^4$ *5.3*	Br $4s^24p^5$ *7.9*	Kr $4s^24p^6$ *10.8*
5	Rb $4d^1$ *-6.9*	Sr $4d^2$ *-10.1*	Y $4d^3$ *-10.8*	Zr $4d^4$ *-9.8*	Nb $4d^5$ *-7.0*	Mo $4d^6$ *-5.3*	Tc $4d^7$ *-6.7*	Ru $4d^8$ *-5.6*	Rh $4d^9$ *-4.8*	Pd $4d^{10}$ *-0.6*	Ag $5s^14d^{10}$ *4.5*	Cd $5s^24d^{10}$ *8.8*	In $5s^25p^1$ *1.4*	Sn $5s^25p^2$ *2.0*	Sb $5s^25p^3$ *3.0*	Te $5s^25p^4$ *3.9*	I $5s^25p^5$ *5.8*	Xe $5s^25p^6$ *8.0*
6	Cs $5d^1$ *-6.4*	Ba $5d^2$ *-9.2*	Lu $5d^3$ *-6.4*	Hf $5d^4$ *-7.9*	Ta $5d^5$ *-7.4*	W $6s^15d^5$ *-3.1*	Re $5d^7$ *-5.1*	Os $5d^8$ *-2.5*	Ir $5d^9$ *-3.1*	Pt $5d^{10}$ *-1.5*	Au $6s^15d^{10}$ *3.7*	Hg $6s^25d^{10}$ *7.5*	Tl $6s^26p^1$ *2.6*	Pb $6s^26p^2$ *3.1*	Bi $6s^26p^3$ *2.7*	Po $6s^26p^4$ *4.1*	At $6s^26p^5$ *4.9*	Rn $6s^26p^6$ *7.3*
7	Fr $6d^1$ *-5.3*	Ra $6d^2$ *-6.4*																
6			La $5d^3$ *-9.8*	Ce $5d^24f^2$ *-11.7*	Pr $5d^24f^3$ *-7.2*	Nd $5d^24f^4$ *-7.2*	Pm $5d^24f^5$ *-6.8*	Sm $5d^24f^6$ *-5.5*	Eu $5d^24f^7$ *-4.2*	Gd $5d^34f^7$ *0.8*	Tb $5d^34f^8$ *1.3*	Dy $5d^24f^{10}$ *-5.0*	Ho $5d^34f^{10}$ *0.8*	Er $5d^24f^{12}$ *-5.8*	Tm $5d^24f^{13}$ *-4.8*	Yb $5d^24f^{14}$ *-2.1*	
7			Ac $6d^3$ *-8.0*		Pa $6d^35f^2$ *-10.8*			Pu $6d^15f^7$ *-9.2*	Am $6d^25f^7$ *-4.1*	Cm $6d^25f^8$ *-5.5*								

Element
ground state atom configuration @ 300 GPa
$\overline{\chi}$

- Polarity inverted intermetallics might be stable
  (Should be observable by electron density measurements)

Ni	Cu
$4s^23d^8$	$4s^13d^{10}$
12.9	*10.2*

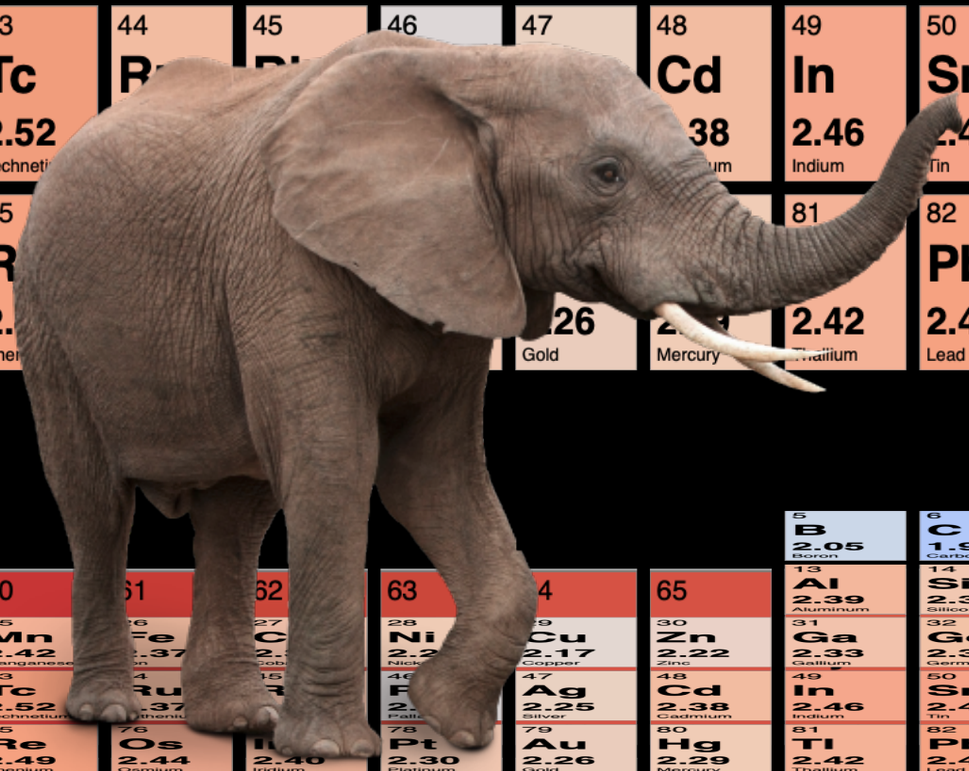
@1atm

CHEMISTRY A European Journal
ChemPubSoc Europe
ChemPhysChem
Articles
doi.org/10.1002/cphc.202000624
Chem Europ European C Societies P
Check for updates

VIP *Very Important Paper*

Non-Bonded Radii of the Atoms Under Compression

Martin Rahm,*[a] Mattias Ångqvist,[b] J. Magnus Rahm,[b] Paul Erhart,[b] and Roberto Cammi[c]



1.3 Å

2.9 Å

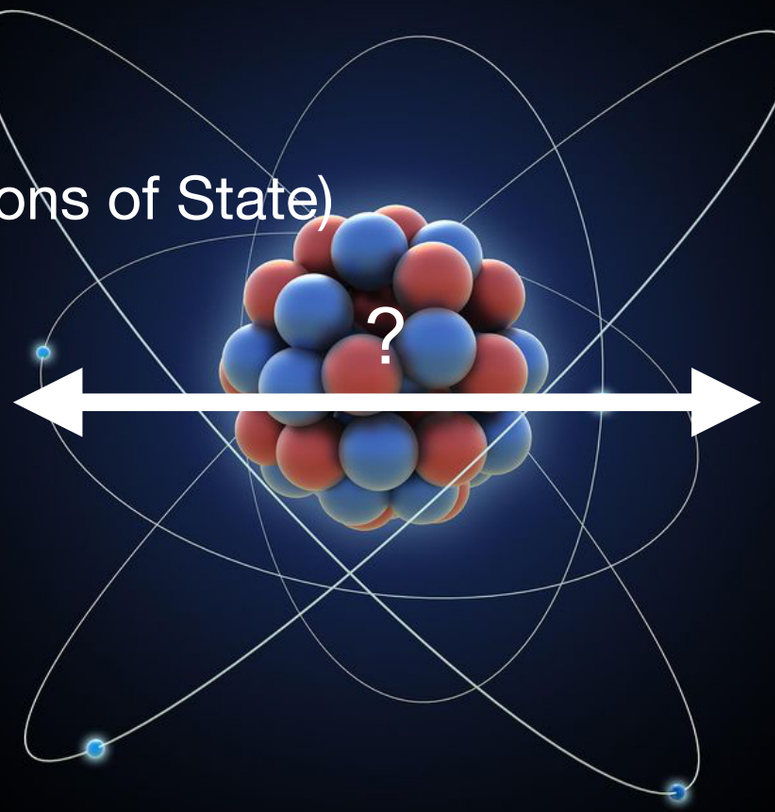
Rahm, M.; Hoffmann, R.; Ashcroft, N. W. Chem. Eur. J. 22, 14625-14632, 2016

Why vdW radii?

- they are useful at ambient conditions
  and allow us to infer:
  - electronic structure
  - atomic interactions
  - size and free space

- under pressure they have been missing!

- are <u>different from bonded</u> radii
  (which can be derived from crystal structures and Equations of State)



Examples of bonded atomic volumes and radii:

D. A. Young, H. Cynn, P. Söderlind, A. Landa, *J. Phys. Chem. Ref. Data* **2016**, *45*, 043101/1-043101/36.

E. B. Royce, *Phys. Rev.* **1967**, *164*, 929-943.

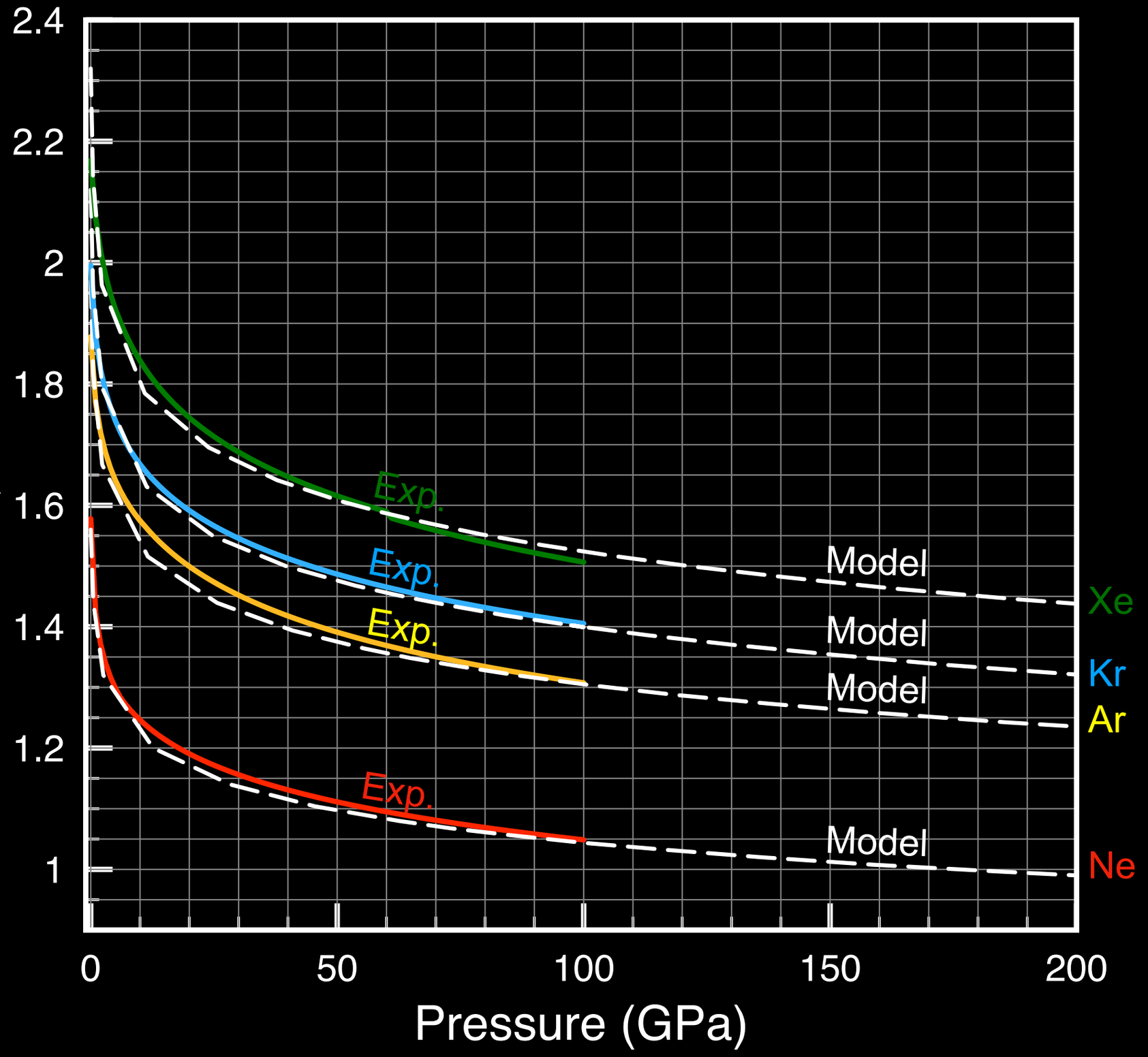
ANDRZEJ WOJCICKI/Getty Images

Model Validation of vdW radii (against noble gas elements)

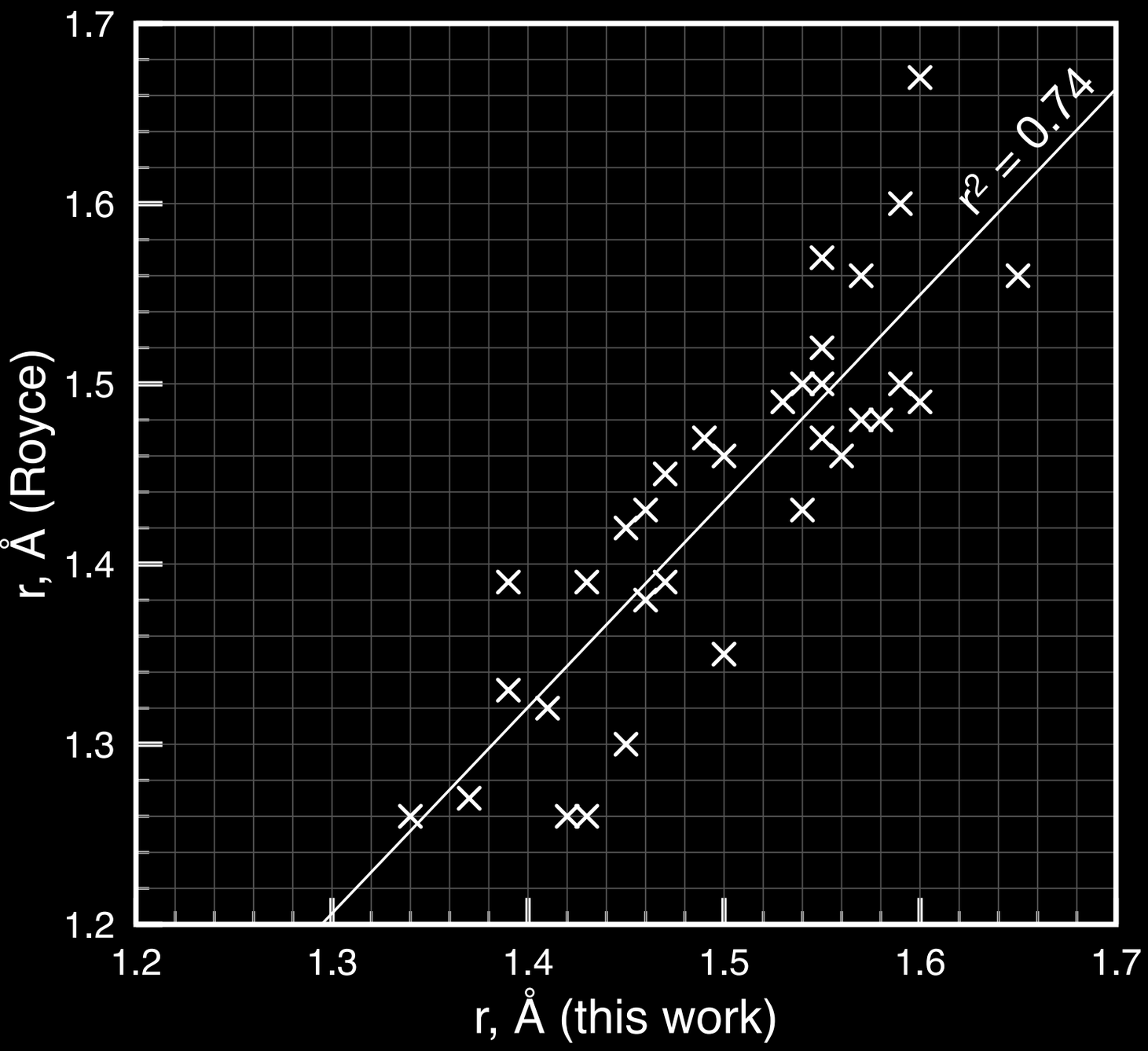
Assuming perfect packing:

$$r(p) = \sqrt[3]{V(p)/4\sqrt{2}}$$

V(p) is the atomic volume

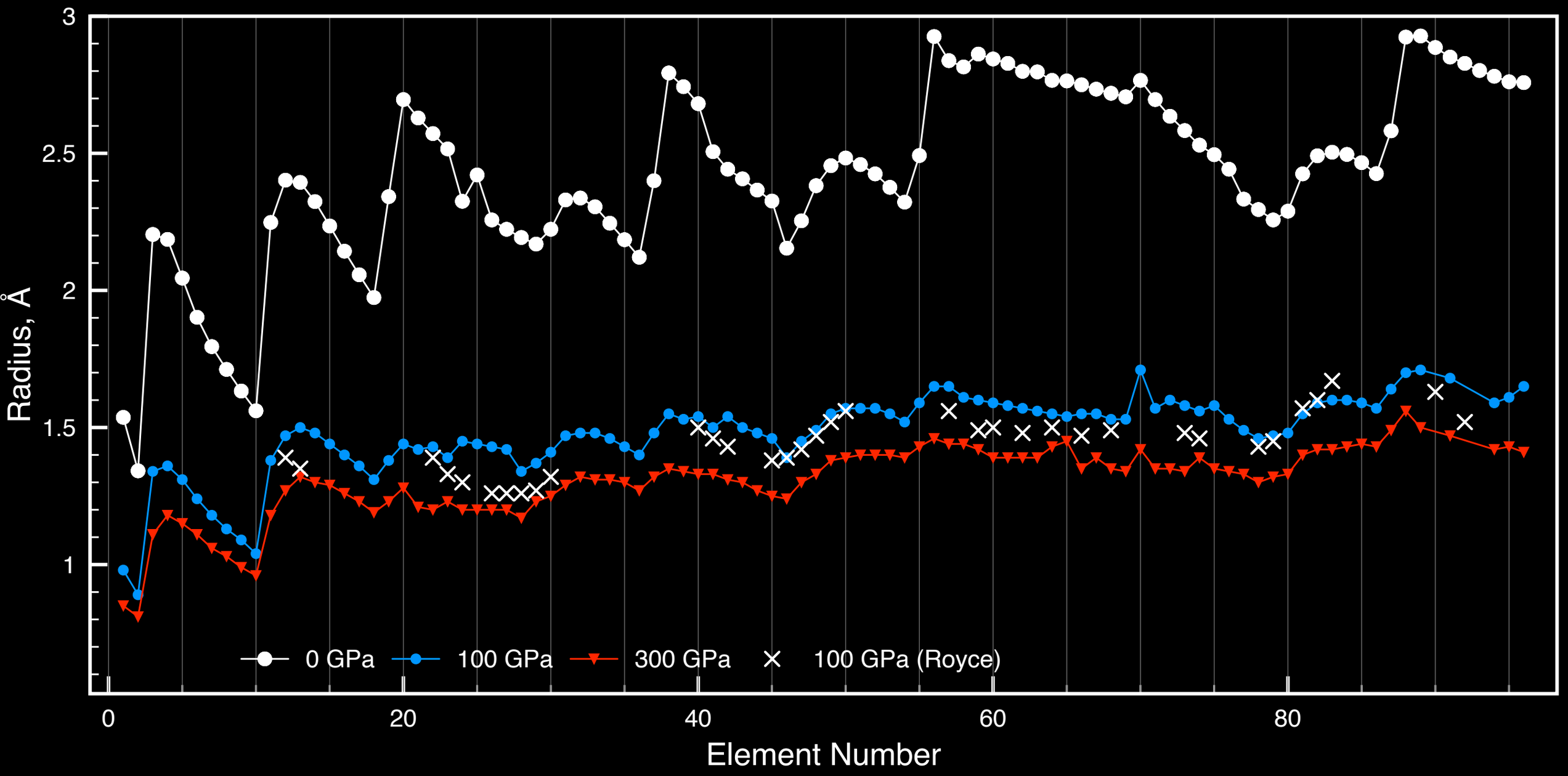


Comparison with 35 Metallic Wigner-Seitz Radii (at 100 GPa)



E. B. Royce, *Phys. Rev.* **1967**, *164*, 929-943.

A first look, at three pressures



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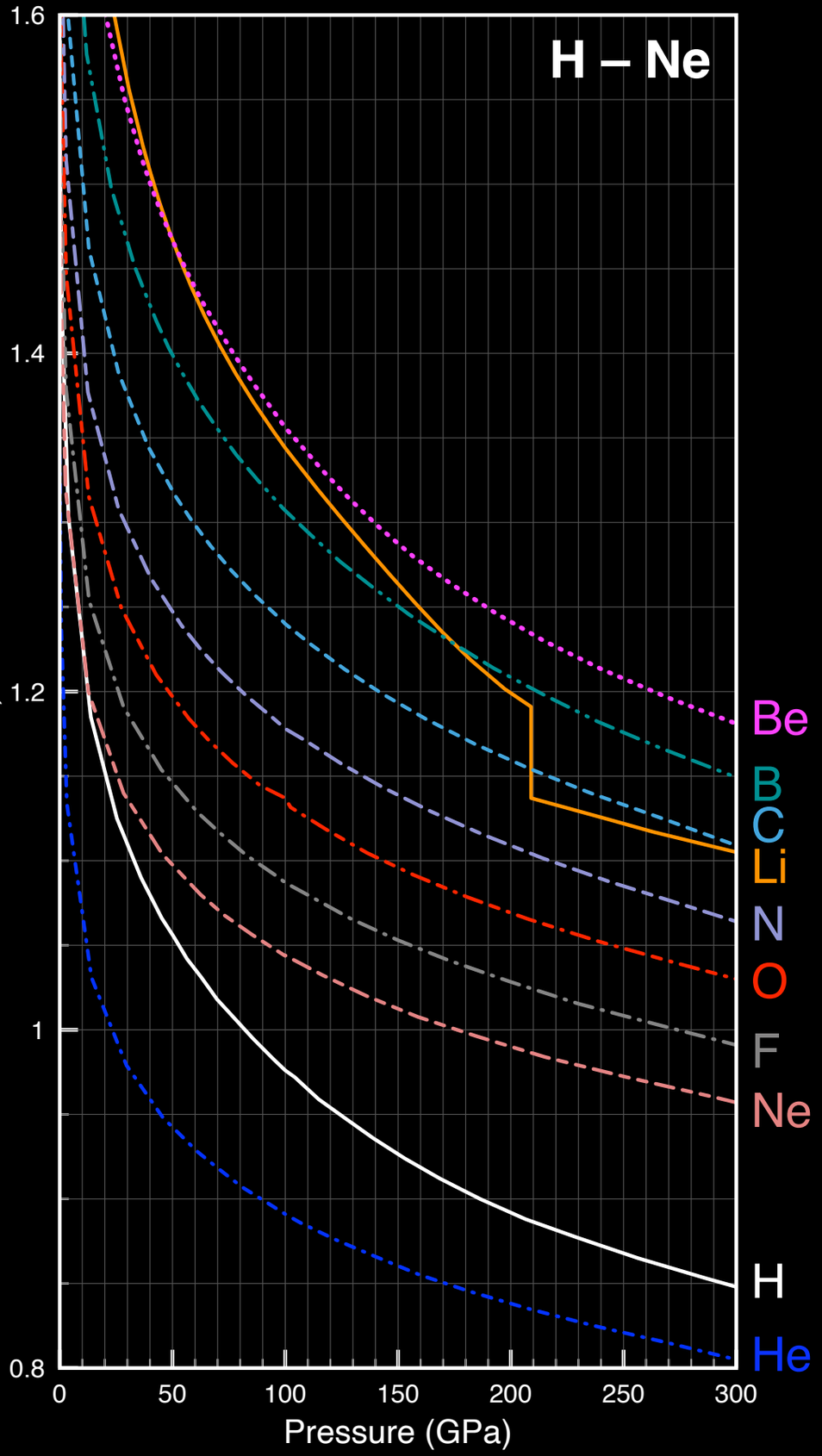

- Atoms are still very different at high pressure
- Relative size ordering can change
- There is something funny going on with Li..

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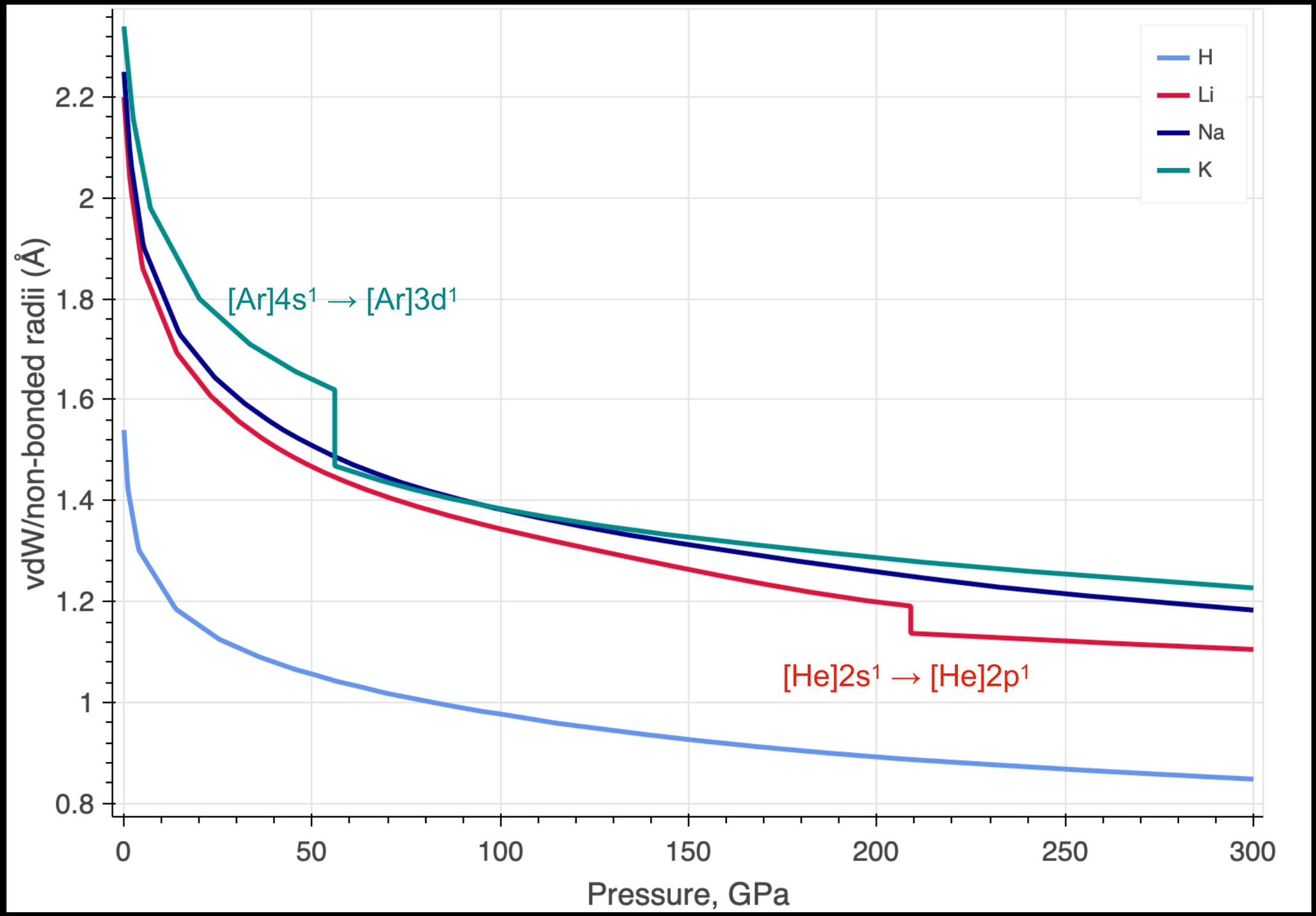
H, Li, Na, K



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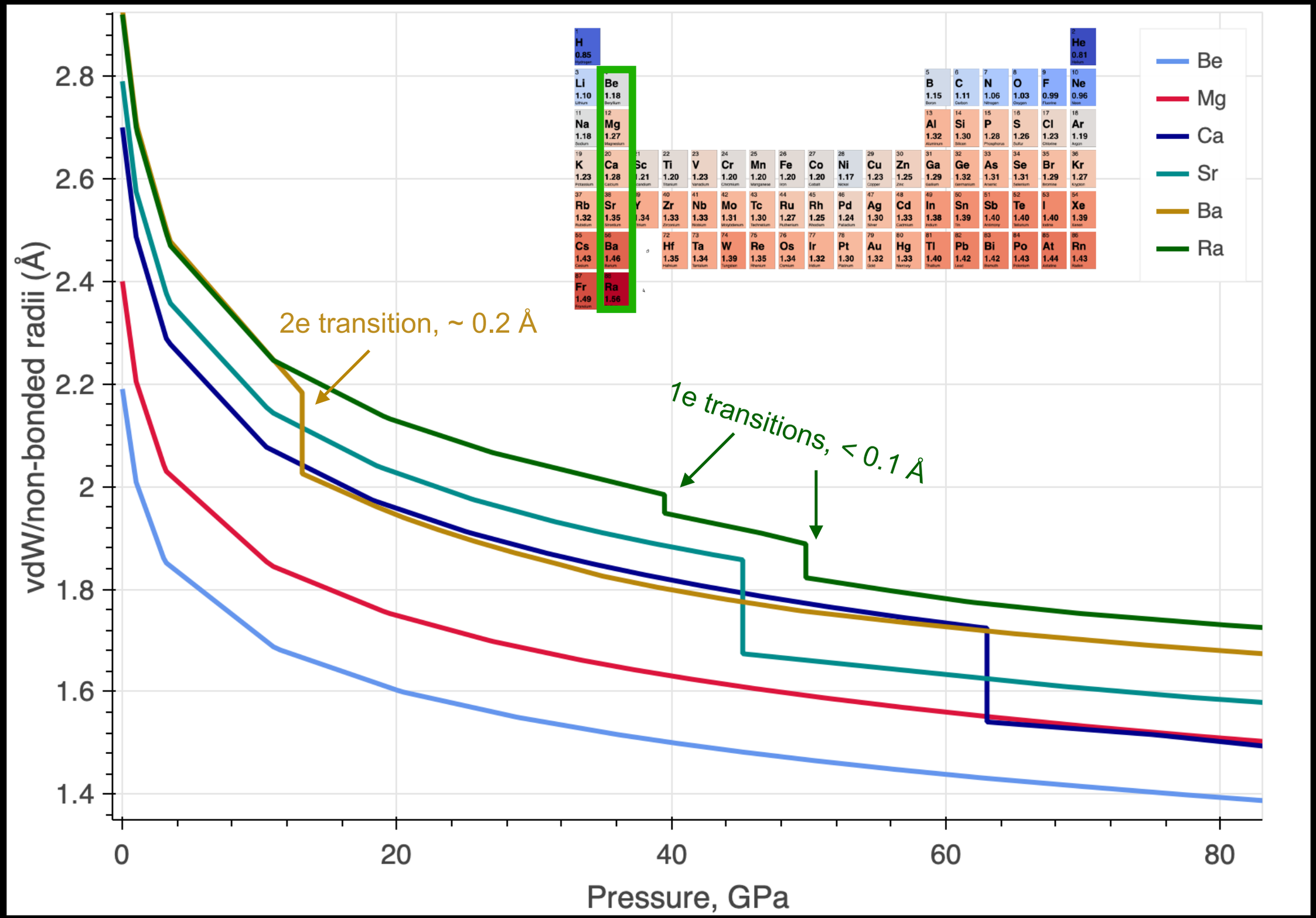
Alkaline Earth Atoms



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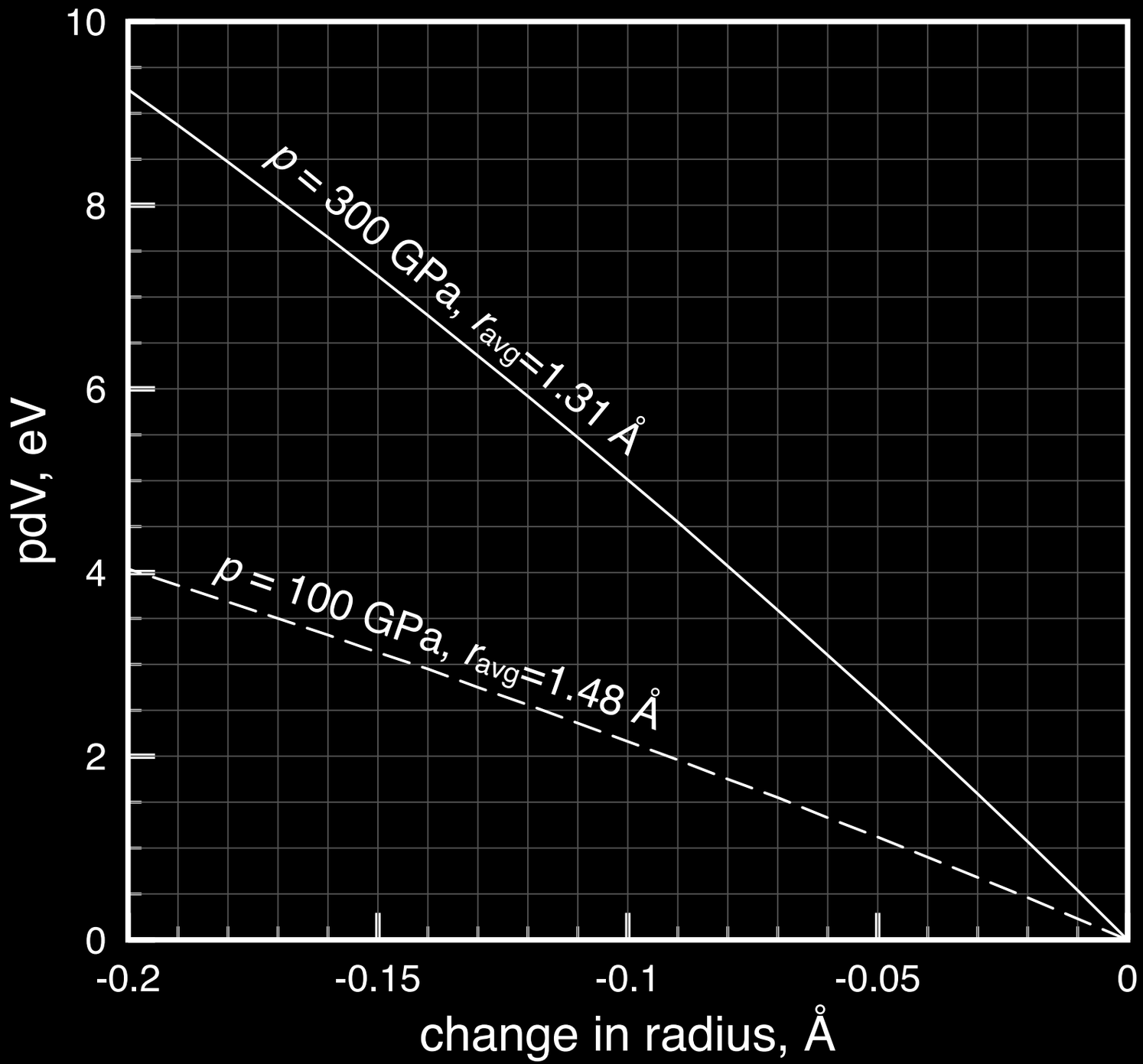
What is 0.1Å worth?



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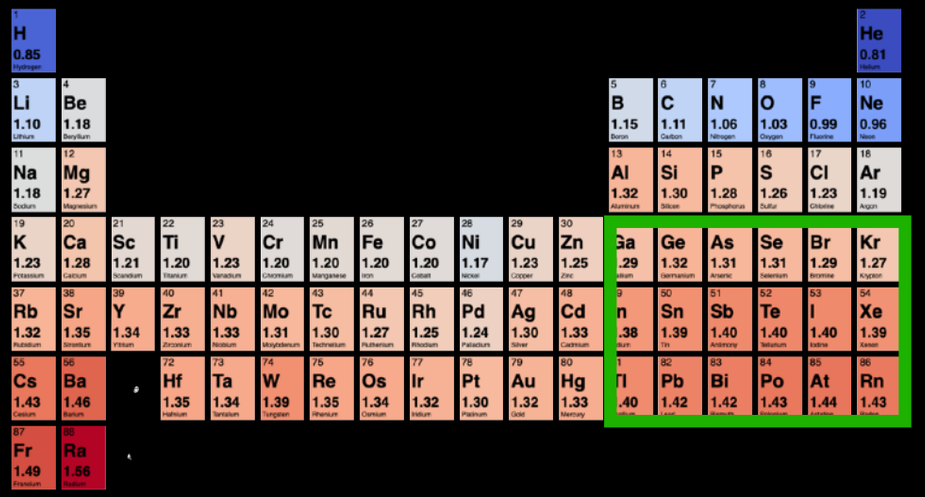
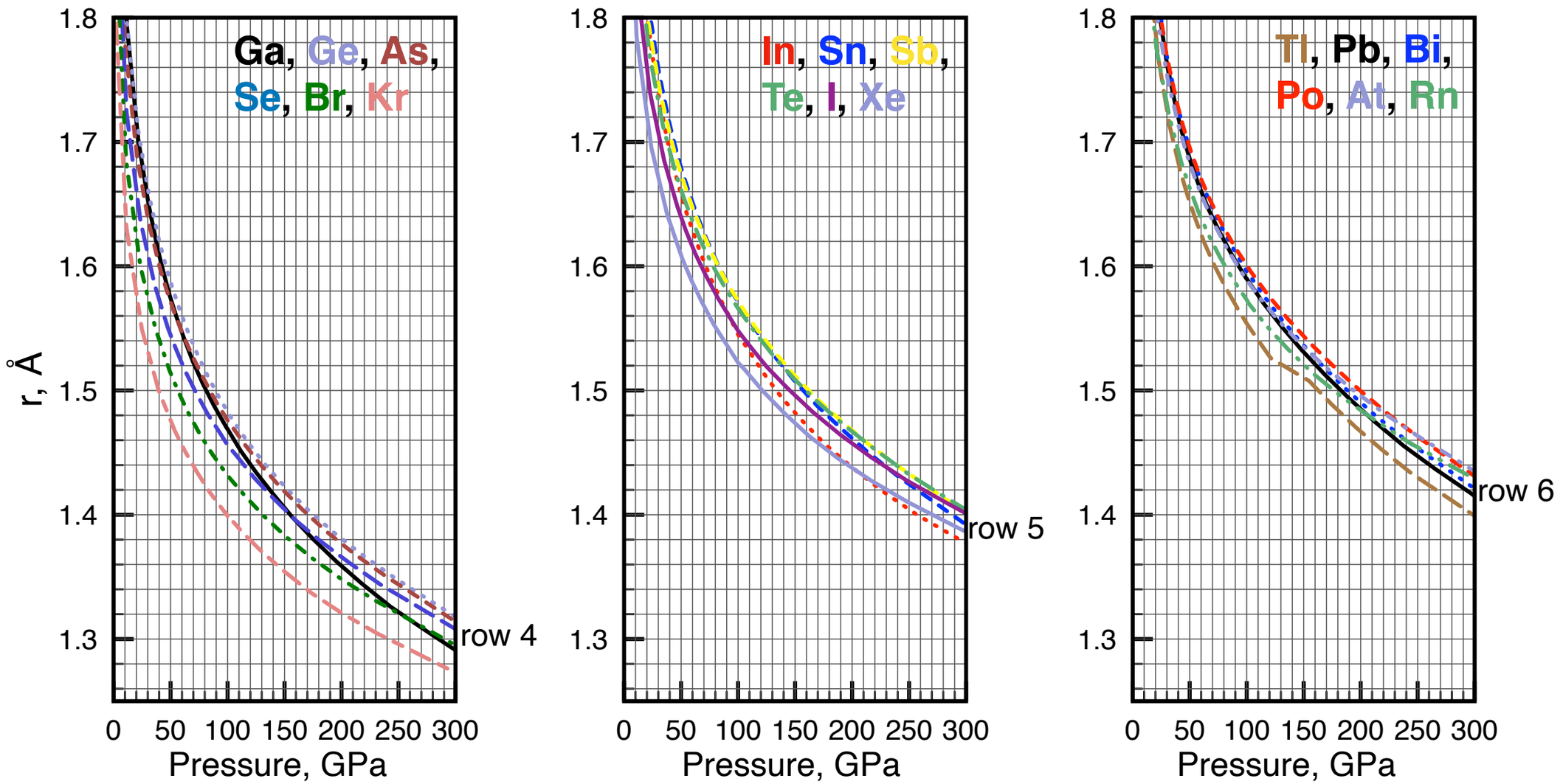
The (Heavy) Main Group

- these rows goes together
- minor changes to relative size ordering





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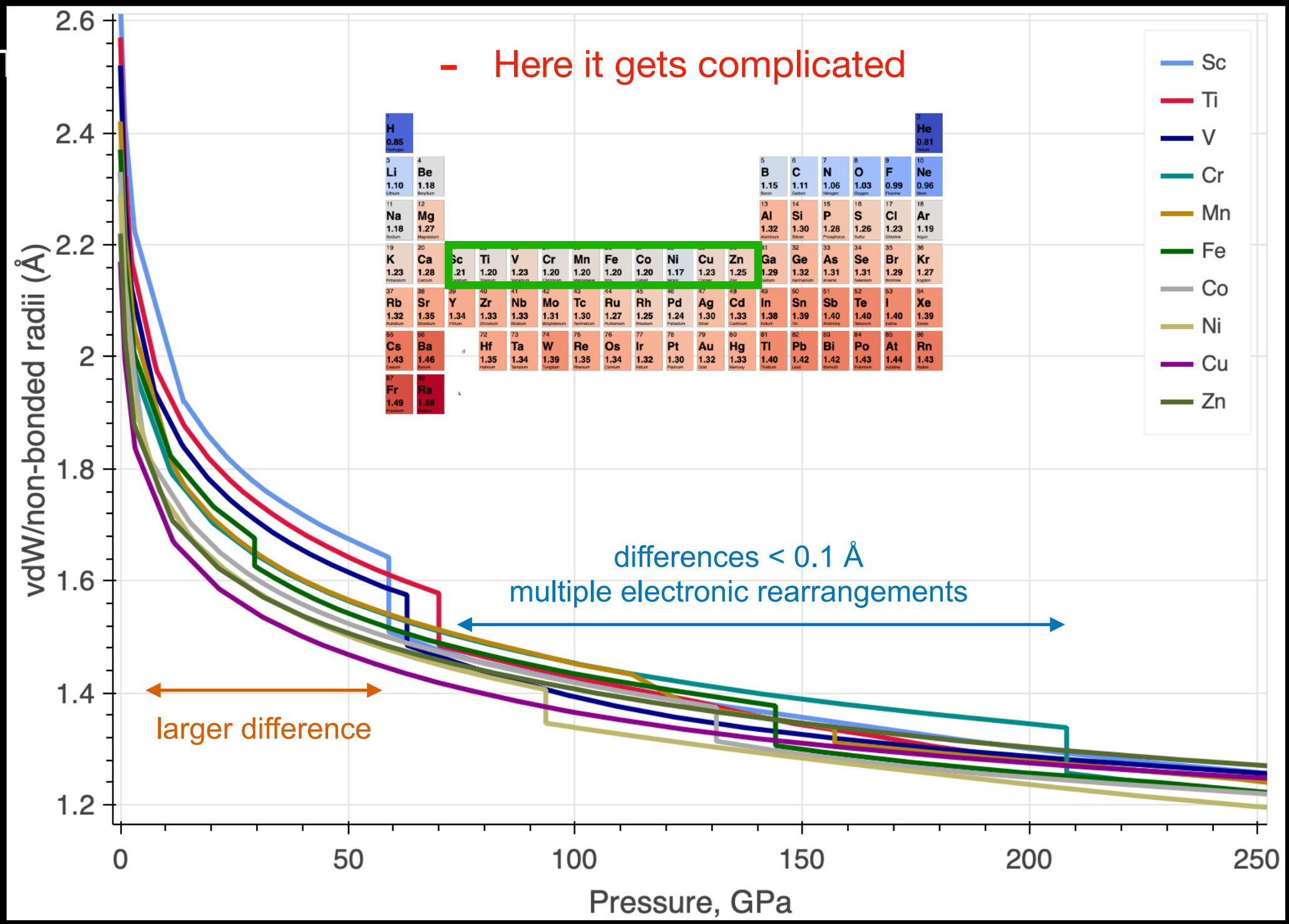
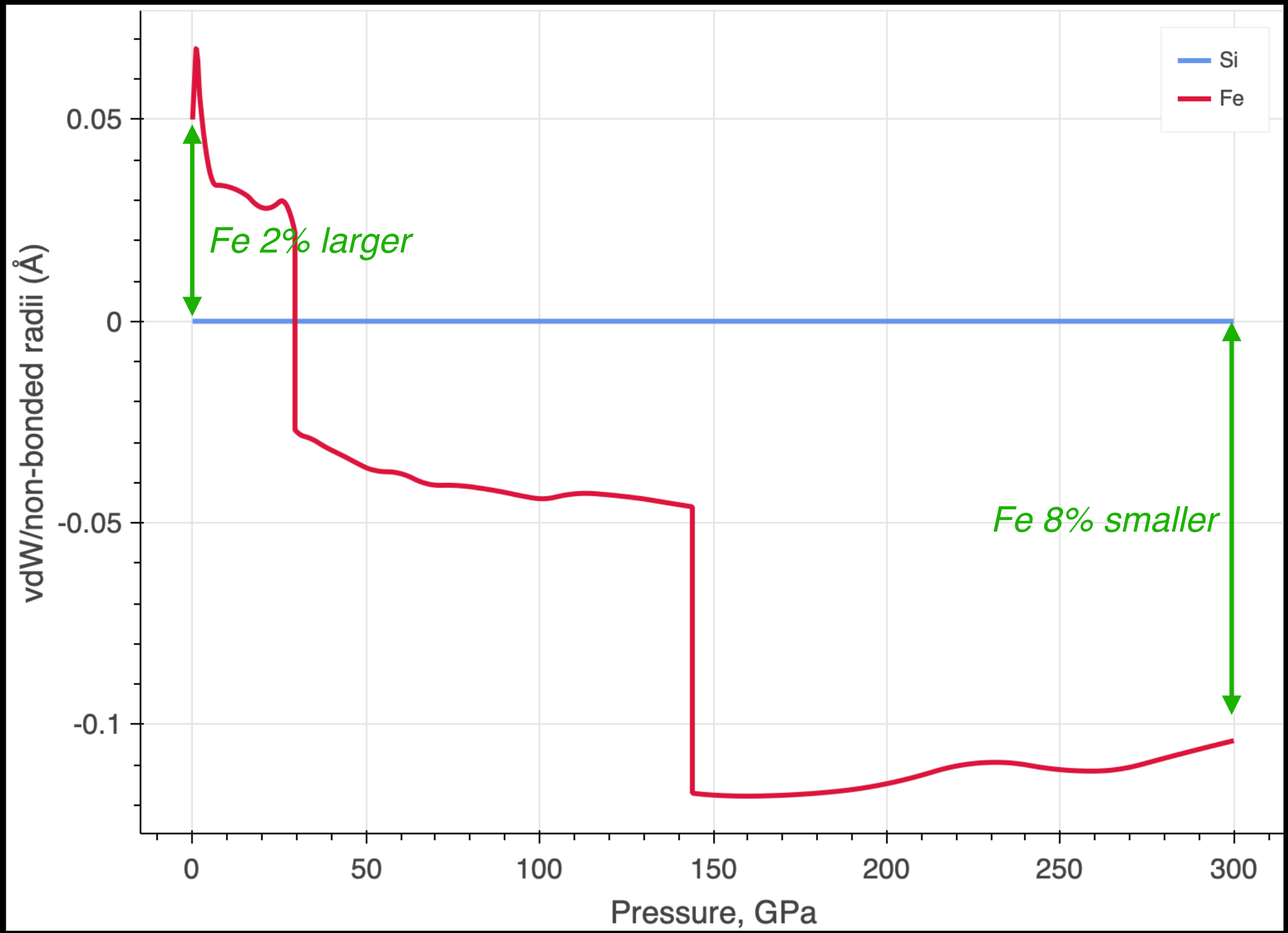
- Here it gets complicated



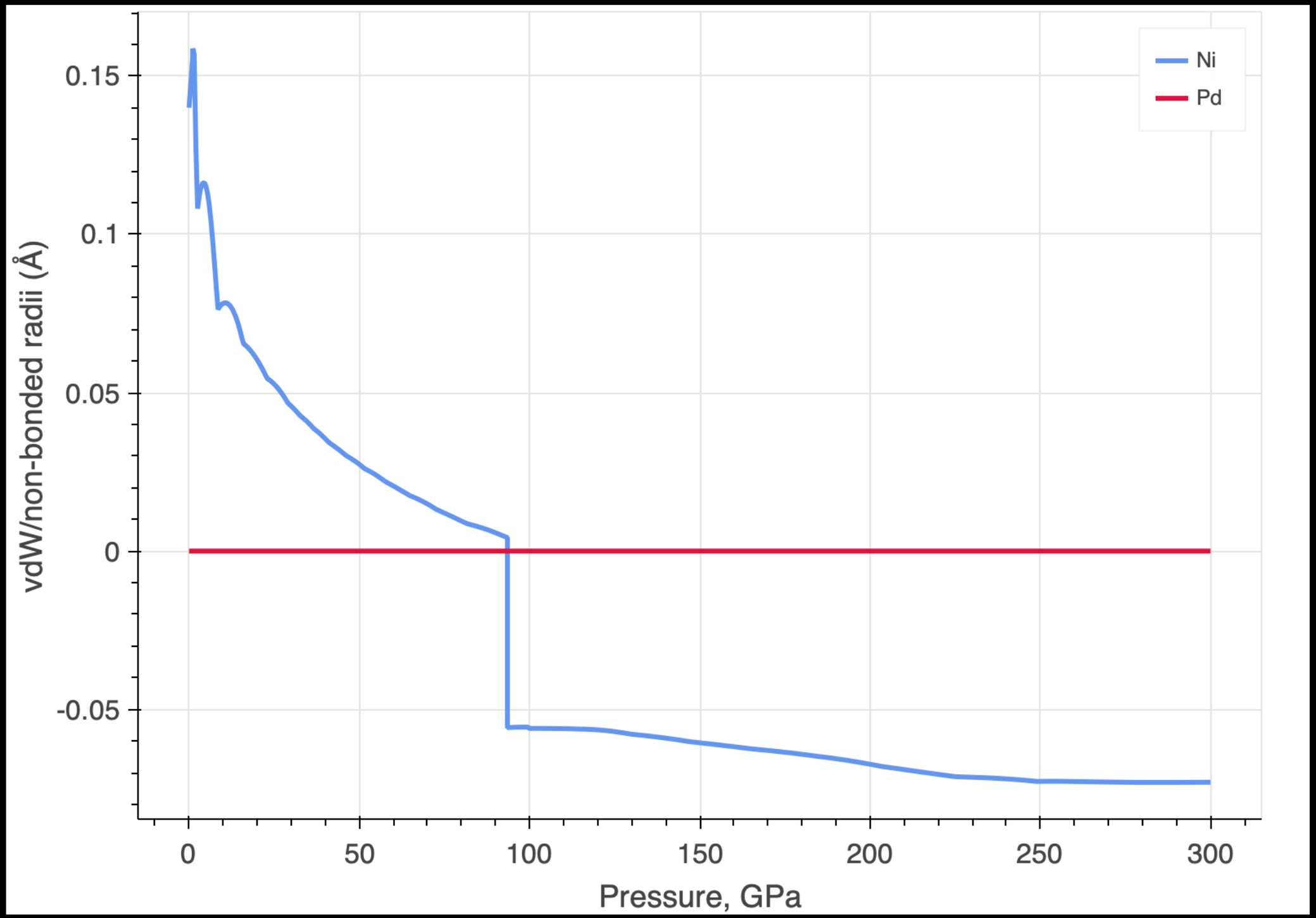
The changes can be dramatic

Radius of Fe relative to Si



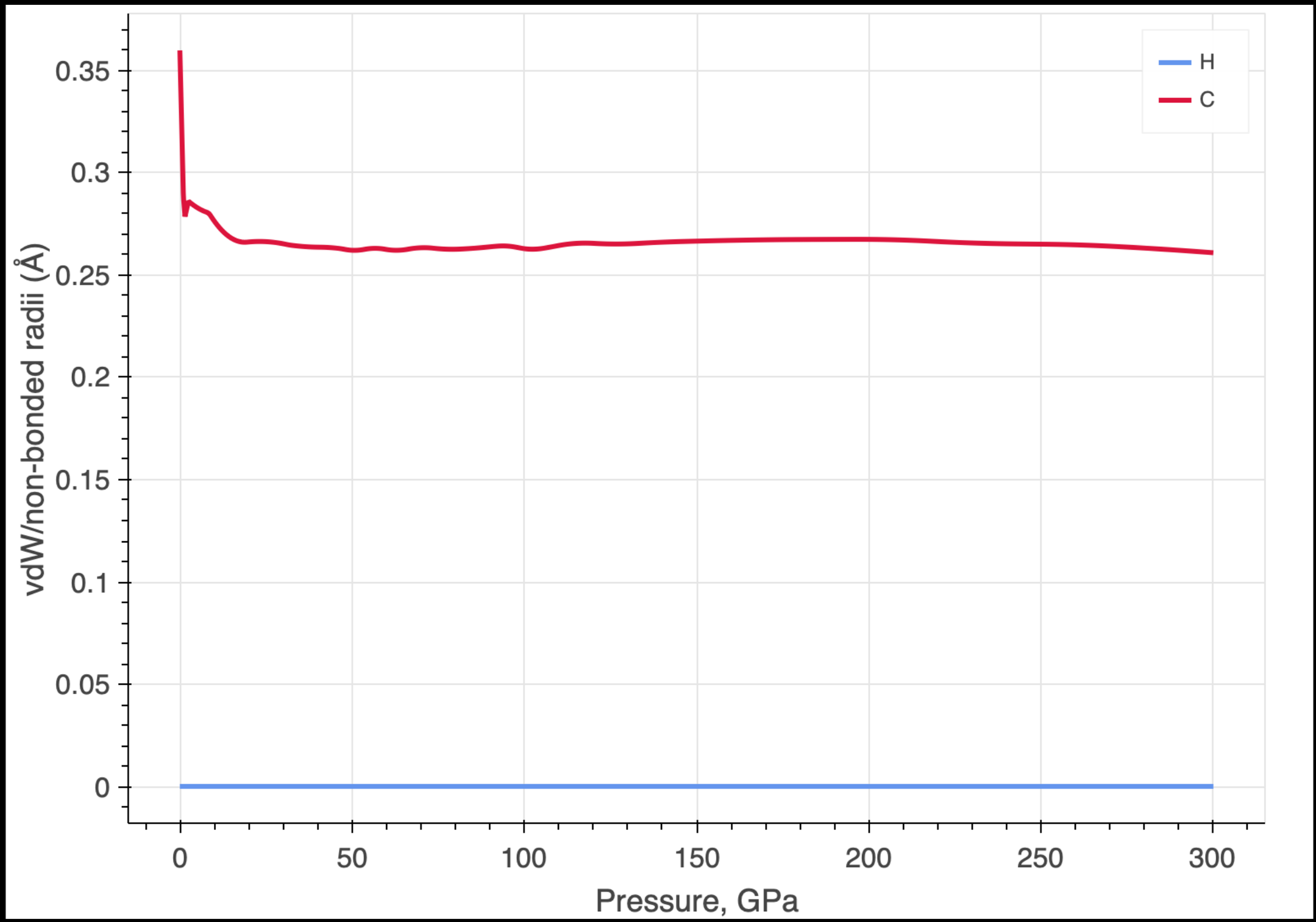
The changes can be dramatic

Radius of Ni relative to Pd



Or not very dramatic at all..

Radius of C relative to H



The vdW radii @ 300 GPa, Å

0.8 Å

1.6 Å

1 H 0.85 Hydrogen																	2 He 0.81 Helium
3 Li 1.10 Lithium	4 Be 1.18 Beryllium											5 B 1.15 Boron	6 C 1.11 Carbon	7 N 1.06 Nitrogen	8 O 1.03 Oxygen	9 F 0.99 Fluorine	10 Ne 0.96 Neon
11 Na 1.18 Sodium	12 Mg 1.27 Magnesium											13 Al 1.32 Aluminum	14 Si 1.30 Silicon	15 P 1.28 Phosphorus	16 S 1.26 Sulfur	17 Cl 1.23 Chlorine	18 Ar 1.19 Argon
19 K 1.23 Potassium	20 Ca 1.28 Calcium	21 Sc 1.21 Scandium	22 Ti 1.20 Titanium	23 V 1.23 Vanadium	24 Cr 1.20 Chromium	25 Mn 1.20 Manganese	26 Fe 1.20 Iron	27 Co 1.20 Cobalt	28 Ni 1.17 Nickel	29 Cu 1.23 Copper	30 Zn 1.25 Zinc	31 Ga 1.29 Gallium	32 Ge 1.32 Germanium	33 As 1.31 Arsenic	34 Se 1.31 Selenium	35 Br 1.29 Bromine	36 Kr 1.27 Krypton
37 Rb 1.32 Rubidium	38 Sr 1.35 Strontium	39 Y 1.34 Yttrium	40 Zr 1.33 Zirconium	41 Nb 1.33 Niobium	42 Mo 1.31 Molybdenum	43 Tc 1.30 Technetium	44 Ru 1.27 Ruthenium	45 Rh 1.25 Rhodium	46 Pd 1.24 Palladium	47 Ag 1.30 Silver	48 Cd 1.33 Cadmium	49 In 1.38 Indium	50 Sn 1.39 Tin	51 Sb 1.40 Antimony	52 Te 1.40 Tellurium	53 I 1.40 Iodine	54 Xe 1.39 Xenon
55 Cs 1.43 Cesium	56 Ba 1.46 Barium		72 Hf 1.35 Hafnium	73 Ta 1.34 Tantalum	74 W 1.39 Tungsten	75 Re 1.35 Rhenium	76 Os 1.34 Osmium	77 Ir 1.32 Iridium	78 Pt 1.30 Platinum	79 Au 1.32 Gold	80 Hg 1.33 Mercury	81 Tl 1.40 Thallium	82 Pb 1.42 Lead	83 Bi 1.42 Bismuth	84 Po 1.43 Polonium	85 At 1.44 Astatine	86 Rn 1.43 Radon
87 Fr 1.49 Francium	88 Ra 1.56 Radium																

57 La 1.44 Lanthanum	58 Ce 1.44 Cerium	59 Pr 1.42 Praseodymium	60 Nd 1.39 Neodymium	61 Pm 1.39 Promethium	62 Sm 1.39 Samarium	63 Eu 1.39 Europium	64 Gd 1.43 Gadolinium	65 Tb 1.45 Terbium	66 Dy 1.35 Dysprosium	67 Ho 1.39 Holmium	68 Er 1.35 Erbium	69 Tm 1.34 Thulium	70 Yb 1.42 Ytterbium	71 Lu 1.35 Lutetium
89 Ac 1.50 Actinium	90 Th - Thorium	91 Pa 1.47 Protactinium	92 U - Uranium	93 Np - Neptunium	94 Pu 1.42 Plutonium	95 Am 1.43 Americium	96 Cm 1.41 Curium							

The vdW radii @ 1atm GPa, Å

1.3 Å

2.9 Å

1 H 1.54 Hydrogen																	2 He 1.34 Helium
3 Li 2.20 Lithium	4 Be 2.19 Beryllium											5 B 2.05 Boron	6 C 1.90 Carbon	7 N 1.79 Nitrogen	8 O 1.71 Oxygen	9 F 1.63 Fluorine	10 Ne 1.56 Neon
11 Na 2.25 Sodium	12 Mg 2.40 Magnesium											13 Al 2.39 Aluminum	14 Si 2.32 Silicon	15 P 2.23 Phosphorus	16 S 2.14 Sulfur	17 Cl 2.06 Chlorine	18 Ar 1.97 Argon
19 K 2.34 Potassium	20 Ca 2.70 Calcium	21 Sc 2.63 Scandium	22 Ti 2.57 Titanium	23 V 2.52 Vanadium	24 Cr 2.33 Chromium	25 Mn 2.42 Manganese	26 Fe 2.37 Iron	27 Co 2.33 Cobalt	28 Ni 2.29 Nickel	29 Cu 2.17 Copper	30 Zn 2.22 Zinc	31 Ga 2.33 Gallium	32 Ge 2.34 Germanium	33 As 2.31 Arsenic	34 Se 2.24 Selenium	35 Br 2.19 Bromine	36 Kr 2.12 Krypton
37 Rb 2.40 Rubidium	38 Sr 2.79 Strontium	39 Y 2.74 Yttrium	40 Zr 2.69 Zirconium	41 Nb 2.51 Niobium	42 Mo 2.44 Molybdenum	43 Tc 2.52 Technetium	44 Ru 2.37 Ruthenium	45 Rh 2.33 Rhodium	46 Pd 2.15 Palladium	47 Ag 2.25 Silver	48 Cd 2.38 Cadmium	49 In 2.46 Indium	50 Sn 2.48 Tin	51 Sb 2.46 Antimony	52 Te 2.42 Tellurium	53 I 2.38 Iodine	54 Xe 2.32 Xenon
55 Cs 2.49 Cesium	56 Ba 2.93 Barium		72 Hf 2.64 Hafnium	73 Ta 2.58 Tantalum	74 W 2.53 Tungsten	75 Re 2.49 Rhenium	76 Os 2.44 Osmium	77 Ir 2.40 Iridium	78 Pt 2.30 Platinum	79 Au 2.26 Gold	80 Hg 2.29 Mercury	81 Tl 2.42 Thallium	82 Pb 2.49 Lead	83 Bi 2.50 Bismuth	84 Po 2.50 Polonium	85 At 2.47 Astatine	86 Rn 2.43 Radon
87 Fr 2.58 Francium	88 Ra 2.92 Radium																

57 La 2.84 Lanthanum	58 Ce 2.82 Cerium	59 Pr 2.86 Praseodymium	60 Nd 2.84 Neodymium	61 Pm 2.83 Promethium	62 Sm 2.80 Samarium	63 Eu 2.80 Europium	64 Gd 2.77 Gadolinium	65 Tb 2.76 Terbium	66 Dy 2.75 Dysprosium	67 Ho 2.73 Holmium	68 Er 2.72 Erbium	69 Tm 2.71 Thulium	70 Yb 2.77 Ytterbium	71 Lu 2.70 Lutetium
89 Ac 2.93 Actinium	90 Th 2.88 Thorium	91 Pa 2.85 Protactinium	92 U 2.83 Uranium	93 Np 2.81 Neptunium	94 Pu 2.78 Plutonium	95 Am 2.76 Americium	96 Cm 2.64 Curium							

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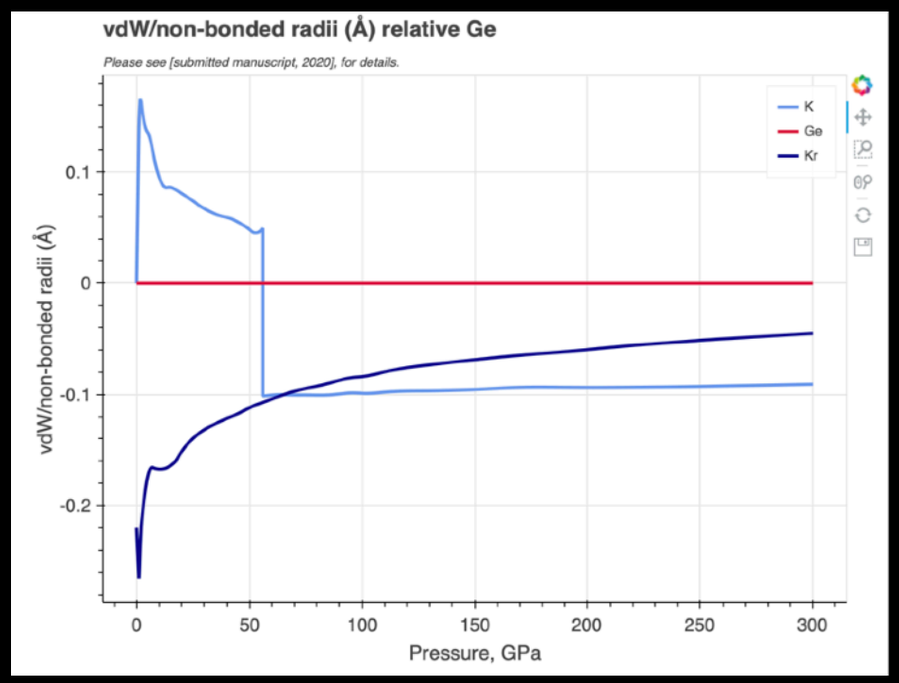
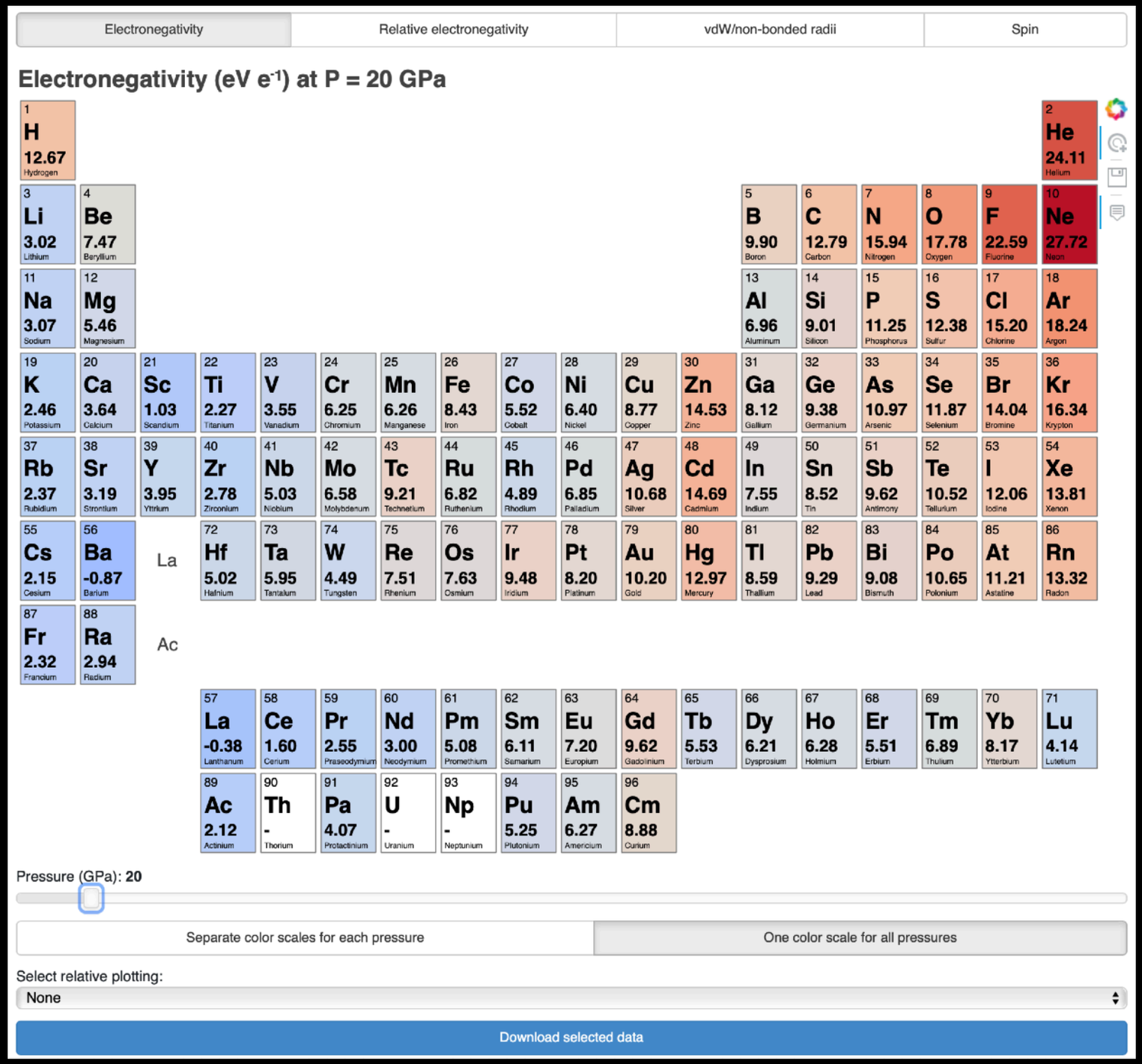
The Atoms Under Pressure Database

https://rahmlab.com/atoms-under-pressure/

- radii
- electronegativity
- electron configuration
- spin

Between 0 to 300 GPa!





Relating Chemical Concepts Using Pressure
(a teaser)

Cite this: *Chem. Sci.*, 2021, **12**, 2397

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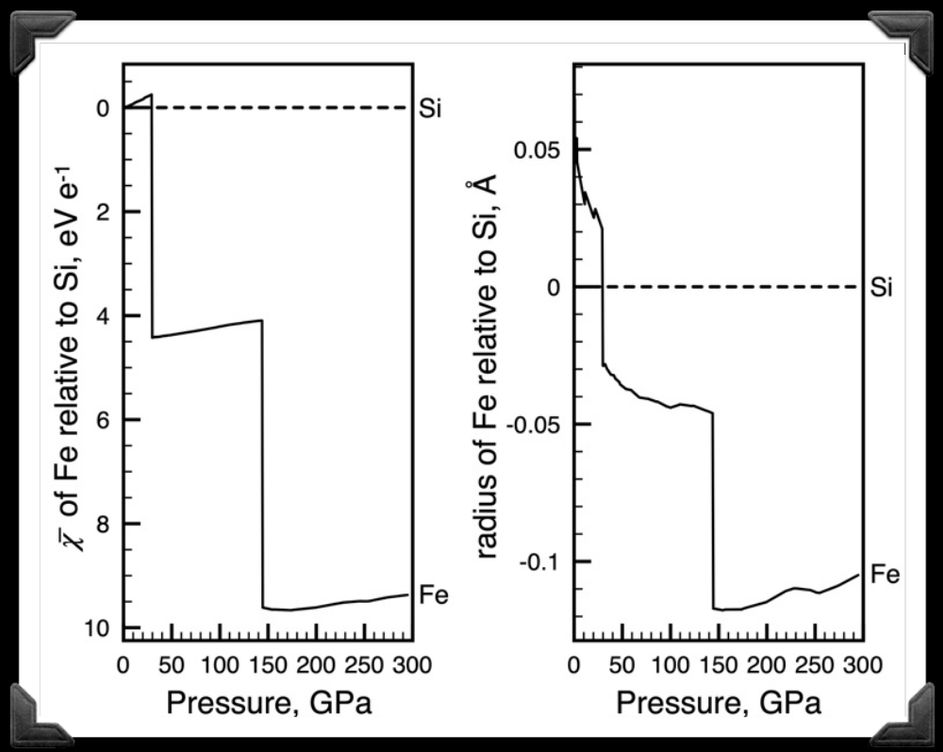
Relating atomic energy, radius and electronegativity through compression

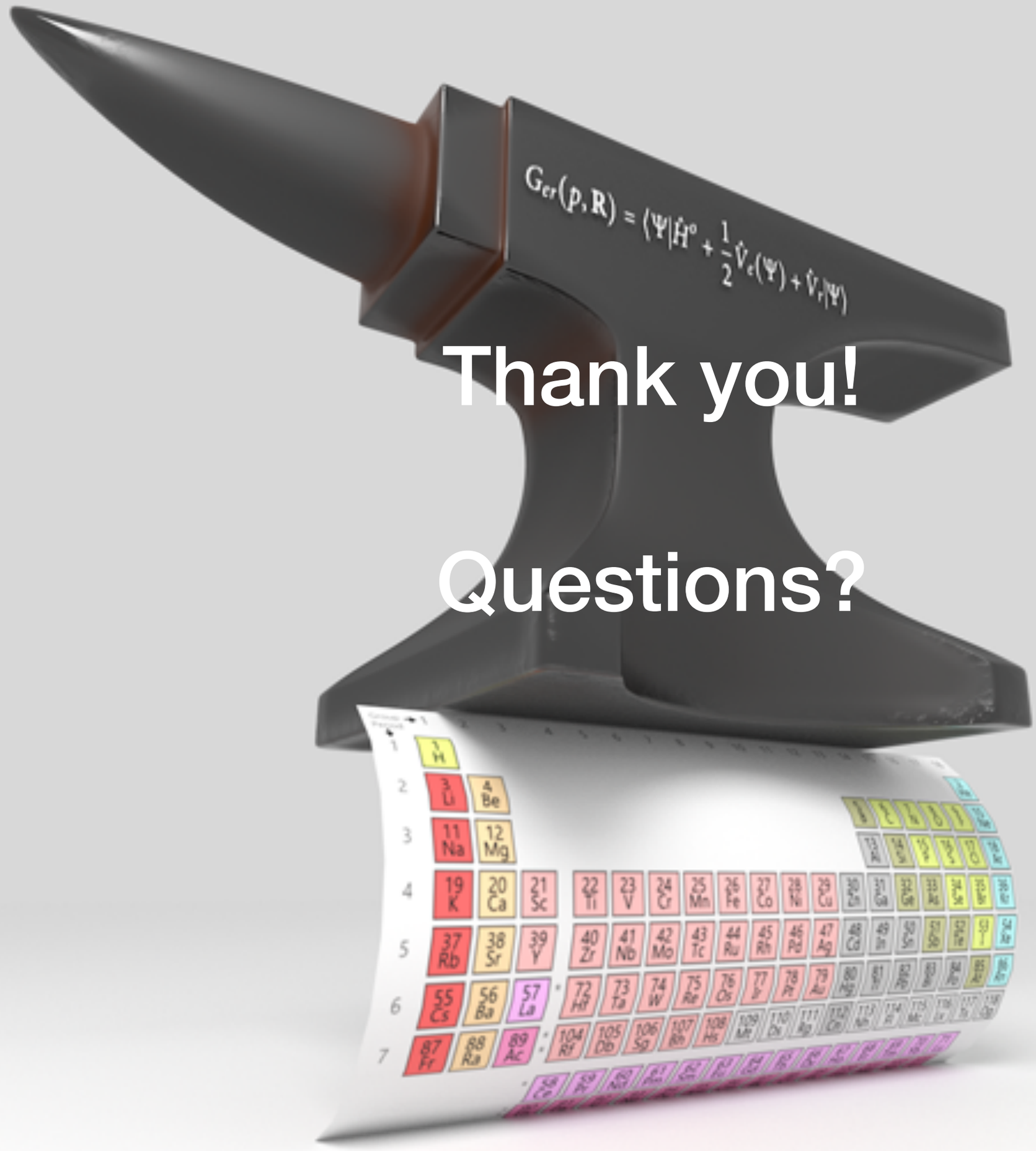
Martin Rahm, *[a] Paul Erhart [b] and Roberto Cammi [c]

Trends in atomic properties are well-established tools for guiding the analysis and discovery of materials. Here, we show how compression can reveal a long sought-after connection between two central chemical concepts – van-der-Waals (vdW) radii and electronegativity – and how these relate to the driving forces behind chemical and physical transformations.



Conclusions

- Ground state electron configurations change with compression
- and so does electronegativity
- as well as the non-bonded radii of the atoms
- Electronic structure of atoms under pressure is predictive of different chemistry
- Radii may be useful in various circumstances (phase transformations, stability, free space, molecularity..)
- The Atoms Under Pressure Database!
- The compressed atom: A key to unlock chemical concepts (teaser)



Thank you!

Questions?