



Understanding Atoms in Tight Places

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CEST Skolkovo July 8th 2021





The Research Group



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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]]







CHALMERS

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)



WACQT

Wallenberg Centre for Quantum Technology

www.wacqt.se





Collaborators & Acknowledgements

Roald Hoffmann Cornell

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Toby Zeng York University

Roberto Cammi

University of Parma



Neil Ashcroft Cornell



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Collaborators & Acknowledgements

Paul Erhart Chalmers

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Magnus Rahm Chalmers

Mattias Ångqvist Chalmers

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





High Pressure Chemistry





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



	1																	18
1	Н 1s ¹																	He 1s ²
	13.6	2											13	14	15	16	17	24.6
2	Li 2s ¹	Be 2s ²	Ele	ectr	one	ega	tivit	ty o	f th	e A	tom	าร	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	0 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	5.4	9.3	Aver	age va	alence	electr	on bine	ding ei	nergy	as T →	• OK		11.4	13.9	16.9	18.0	23.3	28.3
3	Na ^{3s1}	Mg 3s ²	eV e	-1				U U					AI 3s ² 3p ¹	Si 3s ² 3p ²	P 3s ² 3p ³	S 3s ² 3p ⁴	CI 3s ² 3p ⁵	Ar 3s ² 3p ⁶
	5.1	7.6	3	4	5	6	7	8	9	10	11	12	9.1	10.8	12.8	13.6	16.3	19.1
4	4s ¹		Sc 4s ² 3d ¹	Ti 4s ² 3d ²	V 4s ² 3d ³	Cr 4s¹3d⁵	Mn 4s ² 3d ⁵	Fe 4s ² 3d ⁶	Co 4s ² 3d ⁷	Ni 4s ² 3d ⁸	Cu 4s ¹ 3d ¹⁰	Zn 4s ² 3d ¹⁰	Ga ^{4s²4p¹}	Ge ^{4s²4p²}	As 4s ² 4p ³	Se 4s ² 4p ⁴	Br 4s ² 4p ⁵	4s ² 4p ⁶
	4.3	6.1	7.0	8.4	9.7	8.0	12.3	10.1	11.9	12.9	10.2	15.9	9.9	11.1	12.5	13.2	15.2	17.4
5	Rb	Sr 5s ²	Y 5s ² 4d ¹	Zr 5s ² 4d ²	Nb	Mo		Ru 5s14d7	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	1	Xe
5	<i>4.2</i>	5.7	6.3	7.5	7.0	8.3	10.9	8.4	9.3	8.3	12.0	16.1	<i>9.3</i>	10.2	11.2	12.0	13.4	14.9
	Cs	Ba	Lu	Hf	Та	W	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
6	^{6s1} 3.9	^{6s²} 5.2	6s ^{25d1} 6.4	6s ^{25d2} 7.1	6s ² 5d ³ 7.8	6s ² 5d ⁴ 8.6	6s ² 5d ⁵	6s ² 5d ⁶ 9.2	^{6s²5d7} 10.8	^{6s¹5d⁹} 9.5	^{6s¹5d¹⁰} 10.9	^{6s²5d¹⁰ 14.1}	^{6s²6p¹} 10.2	^{6s²6p²} 11.0	^{6s²6p³} 10.7	^{6s²6p⁴} 12.2	^{6s²6p⁵} 12.6	^{6s²6p⁶} 14.6
7	Fr	Ra																
1	4.1	5.3																
			la	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dv	Но	Er	Tm	Yb	El	omont
		6	6s ² 5d ¹	6s ² 4f ¹ 5d ¹	6s ² 4f ³	6s ² 4f ⁴	6s ² 4f ⁵	6s ² 4f ⁶	6s ² 4f ⁷	6s ² 4f ⁷ 5d ¹	6s ² 4f ⁹	6s ² 4f ¹⁰	6s ² 4f ¹¹	6s ² 4f ¹²	6s ² 4f ¹³	6s ² 4f ¹⁴	groun	d state
			6.0	1.3	6./	1.2	1.4	8.3	9.4	13.8	1.1	8.4	8.3	1.6	9.0	10.2	vale	ence
		7	Ac 7s26d1	7s26d2	Pa	U 7e25f36d1	Np	Pu 7s25f6	Am	Cm								
		'	5.8	6.4	6.3	7.5	8.2	7.3	8.3	10.9								ľ
					-													

1 Pauling unit $\approx 6 \text{ eV} \text{ e}^{-1}$

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

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



1																	18
Н ^{1s1} 1 <i>3.6</i>	2											13	14	15	16	17	He ^{1s²} 24.6
Li ^{2s¹} 5.4	Be ^{2s²} 9.3	Ele Aver	ectr	ON alence	electro	tivil	Y O dina er	f th	e A as T →	tom ok	าร	B ^{2s²2p¹ 11.4}	C ^{2s²2p² 13.9}	N ^{2s²2p³ 16.9}	0 ^{2s²2p⁴ 18.6}	F ^{2s²2p⁵ 23.3}	Ne ^{2s²2p⁶ 28.3}
Na ^{3s¹} 5.1	Mg ^{3s²} 7.6	eV e ⁻ 3	-1 4	5	6	7	8	9	10	11	12	Al ^{3s²3p¹} <i>9.1</i>	Si ^{3s²3p²} 10.8	P ^{3s²3p³ 12.8}	S ^{3s²3p⁴} 13.6	CI ^{3s²3p⁵ 16.3}	Ar ^{3s²3p6} 19.1
K ^{4s¹} 4.3	Ca ^{4s²} 6.1	Sc ^{4s²3d¹} 7.0	Ti ^{4s²3d²} <i>8.4</i>	V ^{4s²3d³} <i>9.7</i>	Cr ^{4s¹3d⁵} <i>8.0</i>	Mn ^{4s²3d⁵} 12.3	Fe ^{4s²3d6} 10.1	Co ^{4s²3d⁷} 11.9	Ni ^{4s²3d⁸ 12.9}	Cu ^{4s¹3d¹⁰} 10.2	Zn ^{4s²3d¹⁰} 15.9	Ga ^{4s²4p¹} <i>9.9</i>	Ge ^{4s²4p²} 11.1	As ^{4s²4p³} 12.5	Se ^{4s²4p⁴} 13.2	Br ^{4s²4p⁵} 15.2	Kr ^{4s²4p⁶ 17.4}
Rb ^{5s1} 4.2	Sr ^{5s²} 5.7	Y ^{5s²4d¹} 6.3	Zr ^{5s²4d²} 7.5	Nb ^{5s14d4} 7.0	Mo ^{5s¹4d⁵} <i>8.3</i>	Tc 5s ^{24d^r} 10			T	न	Cd ^{5s²4d¹⁰ 16.1}	5s ²⁵ 9	Sn ^{5s²5p²} 10.2	Sb ^{5s²5p³} 11.2	Te ^{5s²5p⁴} 12.0	I ^{5s²5p⁵} 13.4	Xe ^{5s²5p⁶ 14.9}
Cs ^{6s1} 3.9	Ba ^{6s²} 5.2	Lu ^{6s²5d¹} 6.4	Hf ^{6s²5d²} 7.1	Ta ^{6s²5d³} 7.8	W ^{6s²5d⁴ 8.6}					10.0	- -	TI ^{JS²6p¹ 10.2}	Pb ^{6s²6p²} 11.0	Bi ^{6s²6p³} 10.7	Po 6s ^{26p⁴} 12.2	At ^{6s²6p⁵} 12.6	Rn ^{6s²6p⁶ 14.6}
Fr 7s1 4	Ra ^{7s²}										K						18
¹⁶ , 6 13.6 13.6 13.6 13.6 14.7 14.3 14.3 14.3 14.3 14.3 14.3 14.3 14.3	2 Be 2ª ² 9.3 Mg 7.6 Ca 4 ⁸² 6.1 5 ⁵⁵ 7 Ba ⁶⁵ 2 Ra ⁷⁸ 2 5.3	Ele Aver 3 3 5 5 3 5 5 3 4 4 7.0 5 5 3 4 4 7.0 7 .0 7 .0 7 .0 7 .0 7 .0 7 .0 7	age va 4 4 5 8 4 7 5 6 7 7 7 7 7 7 7 7	5 4823d ² 9.7 55:444 7.0 6625d ³ 7.8	electro 6 48:3d5 58:4d6 58:4d6 8.3 68:5d4 8.6	TIV 7 Nazac 12 10 Gestic 9.7	4 4 10 55 8 6 8 9.2			tor 11 11 4st3dto 10.2 5st4dto 12.0 Au 6st5dto 10.9	12 4s ² 3d ¹⁰ 15. ² 5s ² 4d ¹⁰ 16.1 Hg 6s ² 5d ¹⁰ 14.1	13 28*2p ¹ 11.4 AI 38*3p ¹ Ga 48*4p ¹ 9.9 10.2 10.2	14 C 2s*2p* 13.9 Si 3s*3p* 10.8 Ge 4s*24p* 11.7 So*5p* 10.2 Pb 6s*5p* 11.0	15 N 26 ² 2p ³ 16.9 B 3 ² 2.8 A 4 ² 24p ³ 12.5 A 4 ² 24p ³ 12.5 A 5 ³ 25p ³ 11.2 B 5 ^{525p³} 11.2 B 5 ^{625p³} 10.7	16 2s ² 2p ⁴ 18.6 S 3s ² 3p ⁴ 13.6 S 4s ² 4p ⁴ 13.2 S 5s ² 5p ⁴ 12.0 Po 5s ² 5p ⁴ 12.2	17 F 28*2p ³ C 38*3p ³ C 3 7 7 7 7 7 7 7 7	142 24.6 Ne 28.3 28.3 47 38 ² 3p ³ 79.7 48 ² 4p ⁶ 17.4 Kr 48 ² 4p ⁶ 17.4 8 14.9 Rn 68 ² 6p ⁶ 14.6
	6 7	La 6.0 6.0 5.8	Ce ^{65²4f¹5d¹} 7.3 Th ^{75²6d²} 6.4	Pr 6.24t ³ 6.7 Pa 7s ² 5t ² 6d ¹ 6.3	Nd 6s ² 4t ⁴ 7.2 7.2 7.5	Pm 6s ² 4f ⁵ 7.4 NP 7s ² 5f ⁴ 6d ¹ 8.2	Sm 65 ² 4f ⁶ 8.3 Pu 75 ² 5f ⁶ 7.3	Eu 6s ² 4 <i>t</i> 7 <i>9.4</i> Am 7s ² 5 <i>t</i> 7 <i>8.3</i>	Gd ^{65²4f⁷5d¹ 13.8 Cm ^{75²5f⁷6d¹} 10.9}	ть ^{65²41⁹} 7.7	Dy 6524f ¹¹⁰ 8.4	Ho ^{6s24f11} 8.3	Er ^{6524f12} 7.6	Tm ⁶⁵²⁴¹¹³ 9.0	ҮЬ ^{6в24f14} 10.2		ement i state nce iration

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

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





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

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Non-bonded Radii of the Atoms Under Compression

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4		Full	Paper									5	6	7	8	9	10
ŀ	Be	At	omic	and I	onic I	Radii (of Ele	ment	s 1–96	6		В	С	Ν	0	F	Ne
E	2.19 eryllium	Dr	. Martin I	Rahm ⊠,	Prof. Dr	. Roald F	loffmani	n⊠, Pro	f. Dr. N.	W. Ashcr	oft	2.05 Boron	1.90 Carbon	1.79 Nitrogen	1.71 Oxygen	1.63 Fluorine	1.56 Neon
1	2	Firs	t publishe	ed: 24 Aug	gust 2016	Full public	ation history	,			13	14	15	16	17	18	
	Mg	DO	I: 10.1002	2/chem.20	1602949	View/save o	itation				AI	Si	P	S		Ar	
N	2.40 Nagnesium											2.39 Aluminum	2.32 Silicon	2.23 Phosphorus	2.14 Sulfur	2.06 Chlorine	1.9 7 Argon
2	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
	Ca	Sc	Ti	V	Cr	Mn	Fe	Со	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
	2.70 Calcium	2.63 Scandium	2.57 Titanium	2.52 Vanadium	2.33 Chromium	2.42 Manganese	2.37 Iron	2.33 Cobalt	2.29 Nickel	2.17 Copper	2.22 Zinc	2.33 Gallium	2.34 Germanium	2.31 Arsenic	2.24 Selenium	2.19 Bromine	2.12 Krypton
3	88	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
	Sr	Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	I I	Хе
S	2.79	2.74 Yttrium	2.69 Zirconium	2.51 Niobium	2.44 Molybdenum	2.52 Technetium	2.37 Ruthenium	2.33 Rhodium	2.15 Palladium	2.25 Silver	2.38 Cadmium	2.46 Indium	2.48 Tin	2.46 Antimony	2.42 Tellurium	2.38 Iodine	2.32 Xenon
5	56		72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
	Ba		Hf	Та	W	Re	Os	lr	Pt	Au	Hg	ТІ	Pb	Bi	Ро	At	Rn
	2.93		2.64	2.58	2.53	2.49	2.44	2.40	2.30	2.26	2.29	2.42	2.49	2.50	2.50	2.47	2.43

1.3 Å

2.9 Å

88

Ra

2.92

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

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

1 **H**

1.54 Hydrogen

3 Li 2.20 Lithium 11 Na 2.25 Sodium 19 K 2.34 Potassium

³⁷ **Rb**

2.40 Rubidium

55 **Cs** 2.49 _{Cesium}

87

Fr

2.58 Francium







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



electrostatic and Pauli repulsion with external continuum

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





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**





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?









Method Validation



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





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



The Atoms Under Pressure Database

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

- radii
- electronegativity
- electron configuration
- spin

Between 0 to 300 GPa!



	Elect	ronegativi	ty			Relative e	electroneg	ativity			vdW/	'non-bond	ed radii			Spin	1	
Elect	roneg	jativit	y (eV	e ⁻¹) at	t P = 2	0 GP	а											
1 H 12.67 Hydrogen																	2 He 24.11 Helium	\$ @ =
3 Li 3.02 Lithium	4 Be 7.47 Beryllium											5 B 9.90 Boron	6 C 12.79 _{Carbon}	7 N 15.94 Nitrogen	8 0 17.78 _{Oxygen}	9 F 22.59 Fluorine	10 Ne 27.72 Neon	-
11 Na 3.07 Sodium	12 Mg 5.46 _{Magnesium}											13 AI 6.96 Aluminum	14 Si 9.01 Silicon	15 P 11.25 Phosphorus	16 S 12.38 ^{Sulfur}	17 CI 15.20 Chlorine	18 Ar 18.24 Argon	
19 K 2.46 Potassium	20 Ca 3.64 _{Cakium}	21 Sc 1.03 Scandium	22 Ti 2.27 Titanium	23 V 3.55 Vanadium	24 Cr 6.25 Chromium	25 Mn 6.26 Manganese	26 Fe 8.43	30 Zn 14.53 _{Zinc}	31 Ga 8.12 Gallium	32 Ge 9.38 Germanium	33 As 10.97 Arsenic	34 Se 11.87 Selenium	35 Br 14.04 Bromine	36 Kr 16.34 Krypton				
37 Rb 2.37 Rubidium	38 Sr 3.19 Strontium	39 Y 3.95 Yttrium	40 Zr 2.78 Zirconium	41 Nb 5.03 Nicbium	42 Mo 6.58 Molybdenum	43 TC 9.21 Technetium	44 Ru 6.82 Ruthenium	48 Cd 14.69 _{Cadmium}	49 In 7.55 Indium	50 Sn 8.52 Tin	51 Sb 9.62 Antimony	52 Te 10.52 Tellurium	53 12.06	54 Xe 13.81 _{Xenon}				
55 Cs 2.15 _{Cesium}	56 Ba -0.87 ^{Barium}	La	72 Hf 5.02 Hafnium	73 Ta 5.95 Tantalum	74 W 4.49 Tungsten	75 Re 7.51 Rhenium	76 OS 7.63 _{Osmium}	80 Hg 12.97 Mercury	81 TI 8.59 Thallium	82 Pb 9.29 Lead	83 Bi 9.08 Bismuth	84 PO 10.65 Potonium	85 At 11.21 Astatine	86 Rn 13.32 _{Radon}				
87 Fr 2.32 Francium	88 Ra 2.94 Radium	Ac																-
			57 La -0.38	58 Ce 1.60 _{Cerium}	59 Pr 2.55 Praseodymium	60 Nd 3.00 Neodymium	61 Pm 5.08 Promethium	62 Sm 6.11 Samarium	63 Eu 7.20 Europium	64 Gd 9.62 Gadolinium	65 Tb 5.53 Terbium	66 Dy 6.21 _{Dysprosium}	67 HO 6.28 Holmium	68 Er 5.51 Erbium	69 Tm 6.89 Thulium	70 Yb 8.17 Ytterbium	71 Lu 4.14 Lutetium	
			89 Ac 2.12 Actinium	90 Th - Thorium	91 Pa 4.07 Protactinium	92 U - Uranium	93 Np - Neptunium	94 Pu 5.25 Plutonium	95 Am 6.27 Americium	96 Cm 8.88 Ourium								
Pressure	(GPa): 2	0																
		S	Separate co	olor scales	for each p	oressure						One	color scale	o for all pre	ssures			
Select re	lative plot	ting:																•
								Downloa	d selected	data								



	1																	18
1	Н 1s ¹																	He
	6.1	2											13	14	15	16	17	20.8
2	Li 2p1	Be 2s ²	Ele	ectr	one	gat	tivit	y o	f th	e At	tom	าร	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	O 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	-7.6	-1.3	@ 3	00 GPa	a (eV e	<u>a-1)</u>		-					2.2	6.6	10.8	13.4	18.7	24.4
3	Na 3s1	Mg 3s ²	6 eV	e ⁻¹ ≈ 1	Paulin	g unit							AI 3s²3p¹	Si 3s ² 3p ²	P 3s ² 3p ³	S 3s ² 3p ⁴	CI 3s ² 3p ⁵	Ar 3s ² 3p ⁶
	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	K ^{3d1}		Sc 3d ³		V 3d ⁵		Mn ^{3d7}	Fe ^{3d®}		Ni 3d ¹⁰	Cu 4s ¹ 3d ¹⁰	Zn 4s ² 3d ¹⁰	Ga 4s ² 4p ¹	Ge 4s ^{24p²}	As 4s ² 4p ³	Se 4s ² 4p ⁴	Br 4s ² 4p ⁵	Kr 4s ² 4p ⁶
	-8.5	-11.5	-14.0	-12.5	-10.4	-7.5	-7.7	-9.5	-7.5	-7.1	2.7	8.7	1.5	2.5	4.1	5.3	7.9	10.8
5	Rb 4d1	4d ²	4d ³	Zr 4d⁴	Nb 4d⁵	4d ⁶		4d ⁸	4d ⁹	Pd 4d ¹⁰	Ag 5s ¹ 4d ¹⁰	Cd 5s ² 4d ¹⁰	In 5s²5p¹	Sn ^{5s²5p²}	Sb 5s ² 5p ³	Te 5s²5p⁴	5s²5p⁵	Xe 5s ² 5p ⁶
	-6.9	-10.1	-70.8	-9.8	-7.0	-5.3	-6.7	-5.6	-4.8	-0.6	4.5	8.8	1.4	2.0	3.0	3.9	5.8	8.0
6	Cs ^{5d1}	Ba ^{5d2}	Lu ^{5d³}	Hf ^{5d⁴}	Ta ^{5d⁵}	W 6s¹5d⁵	80 5d7	Os ^{5d®}	5d ⁹	Pt 5d10	Au 6s ^{15d10}	Hg 6s ² 5d ¹⁰	TI 6s²6p¹	Pb 6s ² 6p ²	Bi 6s ² 6p ³	Po 6s ² 6p ⁴	At 6s ² 6p ⁵	Rn 6s²6p ⁶
	-6.4	-9.2	-6.4	-7.9	-7.4	-3.1	-5.1	-2.5	-3.1	-1.5	3.7	7.5	2.6	3.1	2.7	4.1	4.9	7.3
7	Fr ^{6d1} -5.3	Ra ^{6d²} -6.4																
		6	La ^{5d³} -9.8	Ce ^{5d²4f²} -11.7	Pr ^{5d24f3} -7.2	Nd ^{5d24f4} -7.2	Pm ^{5d24f5} -6.8	Sm ^{5d²4f6} -5.5	Eu ^{5d²4f7} -4.2	Gd ^{5d³4f7} <i>0.8</i>	Tb ^{5d³4f⁰} 1.3	Dy ^{5d24f10} -5.0	Ho ^{5d³4f¹⁰} <i>0.8</i>	Er ^{5d24f12} -5.8	Tm ^{5d²4f¹³ -4.8}	Yb ^{5d24f14} -2.1	Ele ground atom con	ement d state figuration
		7	Ac ^{6d³} -8.0		Pa 6d ^{35f2} -10.8			Pu 6d ^{15f7} -9.2	Am ^{6d25f7} -4.1	Cm ^{6d²5f⁸} -5.5							@ 300) GPa

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



	1																	18
1	H 1s ¹																	He
	6.1	2	_										13	14	15	16	17	20.8
2	Li	Be 2s ²	Ele	ectr	one	egat	tivit	y o	f th	e A	tom	าร	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	0 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	-7.0	-1.3	@ 30)0 GPa	a (eV e	} ⁻¹)							2.2	0.0	10.0	13.4	10.7	24.4
3	Na ^{3s1}	Mg ^{3s²}	6 eV	e ⁻¹ ≈ 1	Paulin	ig unit							Al 3s²3p¹	Si ^{3s²3p²}	Р 3s²3p³	S 3s²3p⁴	CI 3s²3p⁵	Ar 3s²3p ⁶
	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	К ^{зd1} <i>-8.5</i>	Ca ^{3d²} - <i>11.5</i>	Sc ^{3d³} -14.0	Ti ^{3d⁴} -12.5	V ^{3d⁵} -10.4	Cr ^{3d⁶} -7.5	Mn ^{3d7} -7.7	Fe ^{3d³} -9.5	Co ^{3d⁹} -7.5	Ni ^{3d¹⁰} -7.1	Cu ^{4s¹3d¹⁰} 2.7	Zn ^{4s²3d¹⁰ <i>8.7</i>}	Ga ^{4s²4p¹} 1.5	Ge ^{4s²4p²} 2.5	As ^{4s²4p³} 4.1	Se ^{4s²4p⁴} 5.3	Br ^{4s²4p⁵} 7.9	Kr ^{4s²4p⁶ 10.8}
5		Sr 4d ²	Y 4d ³	Zr	Nb ₄d⁵	Mo 4d ⁶		Ru ^{4d8}	Rh ^{4d9}	Pd 4d ¹⁰	Ag 5s ¹ 4d ¹⁰	Cd 5s ² 4d ¹⁰	In 5s²5p¹	Sn ^{5s²5p²}	Sb 5s ^{25p³}	Te 5s ² 5p ⁴	5s ² 5p ⁵	Xe 5s ² 5p ⁶
	-6.9	-10.1	-10.8	-9.8	-7.0	-5.3	-6.7	-5.6	-4.8	-0.6	4.5	8.8	1.4	2.0	3.0	3.9	5.8	8.0
6	Cs ^{5d1} -6.4	Ba ^{5d²} -9.2	Lu ^{5d³} -6.4	Hf ^{5d⁴} -7.9	Ta ^{5d⁵} -7.4	₩ ^{6s¹5d⁵} -3.1	Re ^{5d7} -5.1	Os ₅d [®] -2.5	lr ^{5طہ} -3.1	Pt ₅d¹⁰ -1.5	Au ^{6s¹5d¹⁰} <i>3.7</i>	Hg ^{6s²5d¹⁰ 7.5}	TI ^{6s²6p¹} 2.6	Pb ^{6s²6p²} <i>3.1</i>	Bi ^{6s²6p³} 2.7	Po ^{6s²6p⁴} 4.1	At ^{6s²6p⁵ 4.9}	Rn ^{6s²6p⁶ 7.3}
7	Fr -5.3	Ra ^{6d²} -6.4																
		6	La ^{5d³} -9.8	Ce ^{5d²4f²} -11.7	Pr ^{5d²4f³ -7.2}	Nd ^{5d²4f⁴} -7.2	Pm ^{5d²4f⁵} -6.8	Sm ^{5d²4f6} -5.5	Eu ^{5d²4f7} -4.2	Gd ^{5d³4f7} <i>0.8</i>	Тb ^{5d³4f⁸ 1.3}	Dy ^{5d²4f10} -5.0	Ho ^{5d³4f¹0} <i>0.8</i>	Er ^{5d²4f¹²} -5.8	Tm ^{5d²4f¹³ -4.8}	Yb ^{5d24f14} -2.1	ground atom con	ement d state figuration
		7	Ac ^{6d³} -8.0		Pa ^{6d³5f² -10.8}			Pu 6d ^{15f7} -9.2	Am ^{6d25f7} -4.1	Cm ^{6d25f8} -5.5							@ 300 2	GPa

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



	1																	18
1	H 1s ¹																	He 1s ²
	6.1	2											13	14	15	16	17	20.8
2	Li 2p1	Be 2s ²	Ele	ectr	one	gat	tivit	V O	f th	e A [·]	tom	IS	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	O 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	-7.6	-1.3	@ 30	00 GP	a (eV e	g-1)							2.2	6.6	10.8	13.4	18.7	24.4
3	Na 3s1	Mg 3s ²	6 eV	e ⁻¹ ≈ 1	Paulin	g unit							AI 3s ² 3p ¹	Si 3s ² 3p ²	P 3s ² 3p ³	S 3s ² 3p ⁴		Ar 3s ² 3p ⁶
Ŭ	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	K 3d1	Ca 3d ²	Sc 3d ³	Ti 3d⁴	V 3d⁵	Cr 3d ⁶	Mn 3d7	Fe ₃d ⁸	Co	Ni 3d10	Cu 4s13d10	Zn 4s ² 3d ¹⁰	Ga 4s ² 4p ¹	Ge 4s ² 4p ²	As 4s ²⁴ n ³	Se 4s ² 4p ⁴	Br 4s ² 4p ⁵	4s ² 4p ⁶
	-8.5	-11.5	-14.0	-12.5	-10.4	-7.5	-7.7	-9.5	-7.5	-7.1	2.7	8.7	1.5	2.5	4.1	5.3	7.9	10.8
_	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	I	Xe
5	- 6.9	-10.1	-10.8	-9.8	-7.0	- 5.3	- 6 .7	- 5.6	- 4. 8	-0.6	4.5	8.8	1.4	2.0	3.0	3.9	5 s ² 5p ⁵ 5.8	5s ² 5p ⁶ 8.0
	Cs	Ba	Lu	Hf	Та	W	Re	Os	lr	Pt	Au	Hg		Pb	Bi	Ро	At	Rn
6	-6.4	-9.2	-6.4	-7.9	-7.4	-3.1	-5.1	-2.5	- 3 .1	- 1 .5	^{6s¹5d¹⁰ 3.7}	7.5	2.6	<i>3.1</i>	2.7	6s ² 6p ⁴ 4.1	4.9	6s ^{26p⁶} 7.3
7	Fr	Ra																
'	-5.3	<i>-6.4</i>																
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Но	Er	Tm	Yb	Fl	ement
		6	^{5d³}	5d ² 4f ² -11.7	5d ² 4f ³	5d²4f⁴ -7.2	5d²4f⁵ -6.8	^{5d²4f6} -5.5	5d ² 4f ⁷ -4.2	5d ³ 4f ⁷	^{5d³4f®} 1.3	5d ² 4f ¹⁰	5d ³ 4f ¹⁰	5d ² 4f ¹²	5d ² 4f ¹³	5d ² 4f ¹⁴	ground atom con	d state
			Ac		Pa			Pu	Am	Cm							@ 30) GPa
		7	6d ³		6d ³ 5f ²			6d ¹ 5f ⁷	6d ² 5f ⁷	6d ² 5f ⁸								K
					-10.0			-3.2		-3.5							-	

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



	1																	18
1	Н 1s ¹																	He
	6.1	2											13	14	15	16	17	20.8
2	Li ^{2p1}	Be 2s ²	Ele	ectr	one	egat	tivit	y o	f th	e A	tom	IS	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	0 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	-7.0	-1.3	@ 30	00 GPa	a (eV e	e ⁻¹)							2.2	0.0	10.8	13.4	18.7	24.4
3	Na 3s1	Mg ^{3s²}	6 eV	e ⁻¹ ≈ 1	Paulin	ig unit							AI 3s²3p¹	Si ^{3s²3p²}	P 3s ² 3p ³	S 3s²3p⁴	CI 3s²3p ⁵	Ar 3s²3p ⁶
	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	К ^{зd1} -8.5	Ca ^{3d²} -11.5	Sc ^{3d³} -14.0	Ti ^{3d⁴}	V 3d⁵ -10.4	Cr ^{3d⁶} -7.5	Mn ^{3d7} -7.7	Fe ^{3d®} -9.5	Со ^{здэ} -7.5	Ni ^{3d¹⁰} -7.1	Cu ^{4s¹3d¹⁰} 2.7	Zn ^{4s²3d¹⁰ <i>8.7</i>}	Ga ^{4s²4p¹} 1.5	Ge ^{4s²4p²} 2.5	As ^{4s²4p³} 4.1	Se ^{4s²4p⁴} 5.3	Br ^{4s²4p⁵} 7.9	Kr ^{4s²4p⁶ <i>10.8</i>}
	Bb	Sr		7r	Nb	Mo	Tc	Bu	Bh	Pd	Δα	Cd	In	Sn	Sb	Te		Xe
5	^{4d¹} -6.9	4d ² -10.1	4d ³ -10.8	4d⁴ -9.8	^{4d⁵} -7.0	4d ⁶ -5.3	4d ⁷ -6.7	^{4d⁸} -5.6	^{4d9} -4.8	^{4d¹⁰} -0.6	5s ^{14d¹⁰ 4.5}	5s ² 4d ¹⁰ 8.8	^{5s²5p¹} 1.4	^{5s²5p² 2.0}	5s ^{25p³} 3.0	5s ² 5p ⁴ 3.9	5s²5p⁵ 5.8	5s ² 5p ⁶ 8.0
6	Cs	Ba	Lu	Hf	Ta	W	Re	Os	lr	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
o	-6.4	-9.2	-6.4	-7.9	-7.4	-3.1	-5.1	-2.5	- 3 .1	- 1 .5	3.7	7.5	2.6	3.1	2.7	6s²6ρ ⁴ 4.1	4.9	^{δs²δρδ} 7.3
7	Fr ^{6d1} -5.3	Ra ^{6d²} -6.4																
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dv	Но	Er	Tm	Yb	FI	oment
		6	^{5d³} -9.8	5d ² 4f ² -11.7	5d ² 4f ³ -7.2	5d ² 4f ⁴ -7.2	5d ² 4f ⁵ -6.8	^{5d²4f⁶ -5.5}	5d ² 4f ⁷ -4.2	5d ³ 4f ⁷ 0.8	5d ³ 4f ⁸ 1.3	5d ² 4f ¹⁰ -5.0	5d ³ 4f ¹⁰ 0.8	5d ² 4f ¹² -5.8	5d ² 4f ¹³ - 4.8	5d ² 4f ¹⁴ -2.1	ground atom cont	d state
			Ac		Pa			Pu	Am	Cm							@ 300) GPa
		7	6d ³		6d ³ 5f ²			6d15f7	6d ² 5f ⁷	6d25f8							Ī	7
			-8.0		<i>-10.8</i>			-9.2	-4.1	<i>-5.5</i>								L

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



	1																	18
1	H 1s ¹																	He
	6.1	2											13	14	15	16	17	20.8
2	2p ¹	Be 2s ²	Ele	ectr	one	ega	tivit	y o	f th	e At	tom	IS	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	0 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	-7.6	-7.3	@ 30)0 GPa	a (eV e	∋ -1)							2.2	6.6	10.8	13.4	18.7	24.4
3	Na ^{3s1}	Mg 3s ²	6 eV	$e^{-1} \approx 1$	Paulin	ig unit							AI 3s²3p¹	Si 3s²3p²	P 3s ² 3p ³	S 3s²3p4	CI 3s ² 3p ⁵	Ar 3s ² 3p ⁶
	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	K 3d ¹	Ca ^{3d²}	Sc 3d ³	Ti ^{3d⁴}	V 3d⁵		Mn 3d7	Fe ^{3d®}	Co	Ni 3d ¹⁰	Cu 4s ¹ 3d ¹⁰	2n 4s ² 3d ¹⁰	Ga 4s ² 4p ¹	Ge 4s ² 4p ²	As 4s ² 4p ³	Se 4s ² 4p ⁴	Br 4s ² 4p ⁵	Kr 4s ² 4p ⁶
	-8.5	-11.5	-14.0	-12.5	-10.4	-7.5	-7.7	-9.5	-7.5	-7.1	2.7	8.7	1.5	2.5	4.1	5.3	7.9	10.8
5	Rb 4d1	Sr 4d ²	4d ³	Zr 4d⁴	Nb 4d⁵	Mo 4d ⁶	Tc 4d ⁷	Ru	Rh 4d9	Pd 4d10	Ag 5s ¹ 4d ¹⁰	Cd 5s ² 4d ¹⁰	In 5s²5p1	5s ² 5p ²	Sb 5s ² 5p ³	Te 55 ² 50 ⁴	5s²5p⁵	5s ² 5p ⁶
	-6.9	-10.1	-10.8	-9.8	-7.0	-5.3	-6.7	-5.6	-4.8	-0.6	4.5	8.8	1.4	2.0	3.0	3.9	5.8	8.0
	Cs	Ba	Lu	Hf	Та	W	Re	Os	lr	Pt	Au	Hg	TI	Pb	Bi	Ро	At	Rn
6	-6.4	-9.2	-6.4	-7.9	-7.4	6s¹5d⁵ - 3.1	-5.1	-2.5	-3.1	-1.5	^{6s¹5d¹⁰} <i>3.7</i>	6s ² 5d ¹⁰ 7.5	^{6s²6p¹} 2.6	^{6s²6p²} 3.1	6s ² 6p ³ 2.7	6s²6p⁴ 4.1	6s ² 6p ⁵ 4.9	6s ² 6p ⁶ 7.3
7	Fr	Ra																
1	-5.3	<i>-6.4</i>																
				Ce	Dr	Nd	Dm	Sm	Eu	Gd	Th	Dv	Но	Fr	Tm	Yh	EL	omont
		6	5d ³	5d ² 4f ²	5d ² 4f ³	5d ² 4f ⁴	5d ² 4f ⁵	5d ² 4f ⁶	5d ² 4f ⁷	5d ³ 4f ⁷	5d ³ 4f ⁸	5d ² 4f ¹⁰	5d ³ 4f ¹⁰	5d ² 4f ¹²	5d ² 4f ¹³	5d ² 4f ¹⁴	ground	d state
			-9.8	-11.7	-7.2	-1.2	-0.8	-5.5	-4.2	0.8	1.3	-5.0	0.8	-5.8	-4.8	-2.1	atom con	figuration GPa
		7	Ac		Pa			Pu 6d15f7	Am 6d25f7	Cm								
			-8.0		-10.8			-9.2	-4.1	-5.5								ľ

• Lithium becomes a p-block element



	1																	18
1	Н 1s ¹																	He 1s ²
	6.1	2											13	14	15	16	17	20.8
2	2p ¹	Be 2s ²	Ele	ectr	one	egat	tivit	y o	f th	e A	tom	IS	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	0 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	-7.6	-1.3	@ 30)0 GPa	a (eV e	e -1)							2.2	6.6	10.8	13.4	18.7	24.4
3	Na ^{3s1}	Mg 3s ²	6 eV	e ⁻¹ ≈ 1	Paulin	g unit							Al 3s²3p¹	Si ^{3s²3p²}	P 3s ² 3p ³	S 3s²3p4	CI 3s ² 3p ⁵	Ar 3s²3p ⁶
	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	K ^{3d1} -8.5	Ca ^{3d²}	Sc ^{3d³}	Ti ^{3d⁴} -12.5	V 3d⁵ -10 4	Cr ^{3d⁶}	Mn ^{3d7} -77	Fe ^{3d⁸}	Co ^{3d⁹}	Ni ^{3d10} -71	Cu 4s ^{13d10} 27	Zn 4s ² 3d ¹⁰ 87	Ga ^{4s²4p¹} 1.5	Ge ^{4s²4p²} 2.5	As 4s ^{24p³} <i>A</i> 1	Se 4s ² 4p ⁴ 5.3	Br 4s ² 4p ⁵ 79	Kr ^{4s²4p⁶ 10 8}
				7-	Nh			Du										
5	4d ¹	5r 4d ²	4d ³	∠r 4d ⁴ ₋0 2	4d⁵	4d ⁶	4d ⁷	4d ⁸	4d ⁹	4d ¹⁰	Ag 5s ¹ 4d ¹⁰	5s ² 4d ¹⁰	5s²5p¹ 1	5s ² 5p ²	5s ^{25p³}	5s ² 5p ⁴	5s²5p⁵ 5 8	5s ² 5p ⁶
	-0.5	-10.1 De	-10.0	-3.0				-0.0	-7.0	-0.0	7.5					0.3		0.0
6	5d ¹	5d ²	LU 5d ³	HT 5d⁴	Ja 5d⁵	VV 6s¹5d⁵	5d7	5d ⁸	5d ⁹	5d ¹⁰	AU 6s ¹ 5d ¹⁰	Hg 6s ² 5d ¹⁰	6s²6p¹	6s ² 6p ²	BI 6s²6p³	PO 6s²6p⁴	At 6s²6p⁵	6s ² 6p ⁶
	-6.4	-9.2	-6.4	-7.9	-7.4	-3.1	-5.1	-2.5	-3.1	-1.5	3.7	7.5	2.6	3.1	2.7	4.1	4.9	7.3
7	Fr -5.3	Ra ^{6d²} -6.4																
		6	La ^{5d³} -9.8	Ce ^{5d²4f²} -11.7	Pr ^{5d²4f³ -7.2}	Nd ^{5d²4f⁴ -7.2}	Pm ^{5d²4f⁵} <i>-6.8</i>	Sm ^{5d²4f6} -5.5	Eu ^{5d²4f7} -4.2	Gd ^{5d³4f⁷ 0.8}	Tb ^{5d³4f®} 1.3	Dy ^{5d24f10} -5.0	Ho ^{5d³4f¹0} <i>0.8</i>	Er ^{5d24f12} -5.8	Tm ^{5d²4f¹³ -4.8}	Yb ^{5d24f14} -2.1	Ele ground atom con	ement d state figuration
		7	Ac ^{6d³} -8.0		Pa ^{6d³5f²} -10.8			Pu ^{6d15f7} -9.2	Am ^{6d25f7} -4.1	Cm ^{6d25f8} -5.5							@ 300	GPa

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



	1																	18
1	Н 1s ¹																	He 1s ²
	6.1	2											13	14	15	16	17	20.8
2	2p ¹	Be 2s ²	Ele	ectr	one	ega	tivit	y o	f th	e A	tom	าร	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	0 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	-7.6	-1.3	@ 30	00 GPa	a (eV e	€ ⁻¹)							2.2	0.0	10.8	13.4	18.7	24.4
3	Na 3s1	Mg 3s²	6 eV	$e^{-1} \approx 1$	Paulin	ig unit							Al 3s²3p¹	Si ^{3s²3p²}	Р 3s²3p³	S 3s²3p⁴	CI 3s²3p⁵	Ar 3s²3p ⁶
	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	K ^{3d1} -8.5	Ca ^{3d²} -11.5	Sc ^{3d³} -14.0	Ti ^{3d⁴} -12.5	V 3d⁵ -10.4	Cr ^{3d⁶} -7.5	Mn ^{3d7} -7.7	Fe ^{3d®} -9.5	Со ^{здэ} -7.5	Ni ^{3d10} -7.1	Cu ^{4s¹3d¹⁰} 2.7	Zn ^{4s²3d¹⁰ 8.7}	Ga ^{4s²4p¹} 1.5	Ge ^{4s²4p²} 2.5	As ^{4s²4p³} 4.1	Se ^{4s²4p⁴} 5.3	Br ^{4s²4p⁵} 7.9	Kr ^{4s²4p⁶ 10.8}
	Bb	Sr	V	7 r	Nb	Mo	Tc	Bu	Bh	Pd	Δα	Cd	In	Sn	Sb	Te		Xe
5	^{4d¹} -6.9	4d ² -10.1	4d ³ -10.8	4d ⁴ -9.8	^{4d⁵} -7.0	4d ⁶ -5.3	^{4d⁷} -6.7	4d ⁸ -5.6	^{4d9} -4.8	4d ¹⁰ -0.6	^{5s14d10} 4.5	5s ² 4d ¹⁰ 8.8	^{5s²5p¹} 1.4	5s ² 5p ² 2.0	5s ^{25p³} 3.0	5s ² 5p ⁴ 3.9	5s²5p⁵ 5.8	^{5s²5p⁶ 8.0}
ľ	Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
6	^{5d1} -6.4	^{5d²} -9.2	^{5d³} -6.4	^{5d⁴} -7.9	^{5d⁵} -7.4	^{6s¹5d⁵} -3.1	5d ⁷ -5.1	^{5d®} -2.5	5d ⁹ -3.1	^{5d¹⁰} -1.5	^{6s¹5d¹0} 3.7	6s ² 5d ¹⁰ 7.5	^{6s²6p¹} 2.6	6s²6p² 3.1	6s ² 6p ³ 2.7	6s²6p⁴ 4.1	6s²6p⁵ 4.9	6s²6p ⁶ 7.3
7	Fr ^{6d1} -5.3	Ra ^{6d²} -6.4																
					Dre	Mal	Dm	Cm	Eul		Th		На		Tm	Vb		
		6	La ^{5d³}	5d ² 4f ²	5d ² 4f ³	5d ² 4f ⁴	5d²4f⁵ -6.8	5d ^{24f6}	5d ² 4f ⁷ -4.2	5d ³ 4f ⁷	5d ^{34f⁸} 1.3	5d ² 4f ¹⁰	5d ³ 4f ¹⁰	5d ² 4f ¹²	5d ² 4f ¹³ - 4.8	5d ² 4f ¹⁴	ground atom cont	ement state
			Δ		Pa			Pi	Δm	Cm							@ 300) GPa
		7	6d ³		6d ³ 5f ²			6d ¹ 5f ⁷	6d ² 5f ⁷	6d ² 5f ⁸							j	7
			-8.0		-70.8			-9.2	-4.7	-5.5								ما

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



	1																	18
1	H 1s ¹																	He 1s ²
	6.1	2											13	14	15	16	17	20.8
2	Li ^{2p1}	Be 2s ²	Ele	ectr	one	egat	tivit	y o	f th	e A	tom	IS	B 2s ² 2p ¹ 2 2	C 2s ² 2p ² 6 6	N 2s ² 2p ³ 10 8	О 2s ² 2p ⁴ 13 Д	F ₂s²2p⁵ 18 7	Ne ^{2s²2p⁶ 2Л Л}
	-7.0	-1.0	@ 30	00 GPa	a (eV e) ^{−1})								0.0	10.0	10.4	10.1	27.7
3	Na 3s1	Mg 3s ²	6 eV	e ⁻¹ ≈ 1	Paulin	ig unit							3s ² 3p ¹	SI 3s²3p²	Р 3s ² 3p ³	S 3s²3p⁴	CI 3s²3p⁵	Ar 3s²3p ⁶
	-3.3	-2.3	3	4	5	6	1	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	K ^{3d1} -8.5	Ca ^{3d²} -11.5	Sc ^{3d³} -14.0	Ti ^{3d⁴}	∨ _{3d⁵} -10.4	Cr ^{3d⁶} -7.5	Mn ^{3d7} -7.7	Fe ^{3d³} -9.5	Со ^{здэ} -7.5	Ni ^{3d10} -7.1	Cu ^{4s¹3d¹⁰} 2.7	Zn ^{4s²3d¹⁰ <i>8.7</i>}	Ga ^{4s²4p¹} 1.5	Ge ^{4s²4p²} 2.5	As ^{4s²4p³} 4.1	Se ^{4s²4p⁴} 5.3	Br ^{4s²4p⁵} 7.9	Kr ^{4s²4p⁶ <i>10.8</i>}
	Ph	Sr		7r	Nb	Mo	Tc	Bu	Bh	D d	Δα	Cd		Sn	Sh	То		Xe
5	4d ¹ -6.9	4d ²	4d ³	4d ⁴	4d⁵ -7.0	4d ⁶	4d ⁷ -6.7	^{4d®} -5.6	4d ⁹	4d ¹⁰	5s ¹ 4d ¹⁰ 4.5	5s ² 4d ¹⁰ 8.8	5s ² 5p ¹ 1 .4	5s ² 5p ² 2.0	5s ^{25p³} 3.0	5s ² 5p ⁴ 3.9	5s²5p⁵ 5.8	5s ² 5p ⁶
		Ba												 Db				Dn
6	5d ¹	5d ²	5d ³	□ □ □ □ □ □ □ □ □ □	5d⁵	6s¹5d⁵	5d7	5d ⁸	5d ⁹	5d ¹⁰	AU 6s ¹ 5d ¹⁰	ПУ 6s ² 5d ¹⁰	6s ² 6p ¹	6s ² 6p ²	6s ² 6p ³	6s ² 6p ⁴	AL 6s²6p⁵	6s ² 6p ⁶
	-6.4	-9.2	-6.4	-7.9	-7.4	-3.1	-5.1	-2.5	-3.1	-1.5	3.7	7.5	2.6	3.1	2.7	4.1	4.9	7.3
7	Fr ^{6d1} -5.3	Ra ^{6d²} -6.4																
		6	La ^{5d³}	Ce 5d ² 4f ²	Pr 5d ² 4f ³	Nd 5d ² 4f ⁴	Pm 5d ² 4f ⁵	5d ² 4f ⁶	Eu ^{5d²4f7}	Gd 5d ³ 4f ⁷	Tb 5d ³ 4f ⁸	Dy 5d ² 4f ¹⁰	Ho 5d ³ 4f ¹⁰	Er 5d ² 4f ¹²	Tm 5d ² 4f ¹³	Yb 5d ² 4f ¹⁴	El ground	ement
			-9.8	-11.7	-1.2	-1.2	-6.8	-5.5	-4.2	0.8	1.3	-5.0	0.8	-5.8	-4.8	-2.1	atom con	figuration
		7	Ac		Pa			Pu	Am	Cm							@ 30	
		1	-8.0		-10.8			-9.2	-4.1	-5.5								ľ

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





	1																	18
1	H 1s ¹																	He
	6.1	2											13	14	15	16	17	20.8
2	Li ^{2p1} -76	Be 2s ² -1.3	Ele	ectr	one	egat	tivit	y o	f th	e A	tom	IS	B 2s ² 2p ¹ 2 2	C 2s ² 2p ² 66	N 2s ² 2p ³ 10 8	0 2s ² 2p ⁴ 1.3 4	F ²s²2p⁵ 18 7	Ne 2s ² 2p ⁶ 24 4
			@ 3(JO GP	a (ev e	; -1)												
3	Na 3s1	NIG 3s ²	6 eV	e ⁻¹ ≈ 1	Paulin	g unit							AI 3s ² 3p ¹	3s ² 3p ²	2 3s ² 3p ³	3s²3p4	3s ² 3p ⁵	Ar 3s ² 3p ⁶
	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9,3	13.3
4	K 3d ¹	Ca ^{3d²}	Sc 3d ³	Ti 3d ⁴	V 3d⁵	Cr 3d ⁶	Mn ^{3d7}	Fe ^{3d⁸}	Co 3d ⁹	Ni 3d ¹⁰	Cu 4s ¹ 3d ¹⁰ 2 7	Zn 4s ² 3d ¹⁰ 97	Ga ^{4s²4p¹}	Ge 4s ^{24p²} 2 5	As 4s ² 4p ³ 1	Se 4s ² 4p ⁴ 5 2	Br 4s ² 4p ⁵ 7 0	Kr 4s ² 4p ⁶
	-0.5	-11.5	-14.0	-12.5	-10.4	-7.5		-9.5	-7.5	-/./	2.1	0.7	1.5	2.5	4.1	5.5	13	10.0
5	Rb 4d1	4d ²	4d ³	Zr ₄d⁴	Nb 4d⁵	4d ⁶	4d7	80 4d ⁸	4d ⁹	Pd 4d ¹⁰	Ag 5s¹4d¹⁰	5s ² 4d ¹⁰	5s²5p¹	5s ^{25p²}	Sb 5s ² 5p ³	Te 5s²5p⁴	5s²5p⁵	Xe 5s ² 5p ⁶
	-6.9	-10.1	-10.8	-9.8	-7.0	-5.3	-6.7	-5.6	-4.8	-0.6	4.5	8.8	1.4	2.0	3.0	3.9	5.8	8.0
6	Cs	Ba	Lu	Hf	Ta	W	Re	Os	١r	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
O	-6.4	- 9.2	-6.4	- 7.9	-7.4	-3.1	-5.1	-2.5	-3.1	-1.5	<i>3.7</i>	7.5	<i>2.6</i>	3.1	2.7	4.1	4.9	7.3
_	Fr	Ra																
1	-5.3	-6.4																
			La	Ce	Dr	Nd	Pm	Sm	Eu	Gd	Tb	Dv	Но	Fr	Tm	Yb	EL	mont
		6	5d ³	5d ² 4f ²	5d ² 4f ³	5d ² 4f ⁴	5d²4f⁵ -6 8	5d ² 4f ⁶	5d ² 4f ⁷	5d ³ 4f ⁷	5d ³ 4f ⁸ 1.3	5d ² 4f ¹⁰	5d ³ 4f ¹⁰	5d ² 4f ¹²	5d ² 4f ¹³ - 4 8	5d ² 4f ¹⁴	ground	d state
																	@ 300) GPa
		7	6d ³		6d ³ 5f ²			6d15f7	AIN 6d ² 5f ⁷	6d ² 5f ⁸							ī	
			-8.0		-10.8			-9.2	-4.1	-5.5								L

• It is "easier" to fluorinate... <u>anything</u> under pressure.



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

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 NaCl₃, 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 IF₈ 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 pentagonalbiypyramidal 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 IF₅ and I₂ (140 GPa). The team also discovered new species that are thermodynamically stable at 300 GPa. These include IF₈ as well as the higher fluorides IF₁₀, IF₁₁ and IF₁₂ that also feature octacoordinate I on account of having 'free' F₂ in their lettices

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, and higher-lying t_{2a} sets, can overlap with filled F-centred orbitals in an interaction familiar to inorganic chemists.

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 IF₈, a truly hypervalent molecule. At ambient pressure, the anion [IF₈]⁻ 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 [IF₈]⁻ hypervalent.

Yang and co-workers acquired independent evidence for the involvement of 5d orbitals in the bonding of IF₈ 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, is metallic and has F-centred vacancies. Thus, IF₈ 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

 $\label{eq:order} \begin{array}{l} \textbf{ORIGINAL ARTICLE Luo, D. et al. A hypervalent} \\ \text{and cubically coordinated molecular phase of IF}_{s} \\ \text{predicted at high pressure. Chem. Sci. https://doi.} \\ \text{org/10.1039/C8SC04635B (2019)} \end{array}$

Sredit: David Schilter/Springer Nature Limited





	1																	18
1																		He
	6.1	2							_				13	14	15	16	17	20.8
2	Li ^{2p1}	Be 2s ²	Ele	ectr	one	ega	tivit	y o	f th	e A	tom	IS	B 2s ² 2p ¹	C 2s ² 2p ²	N 2s ² 2p ³	0 2s ² 2p ⁴	F 2s ² 2p ⁵	Ne 2s ² 2p ⁶
	-7.0	-1.3	@ 30)0 GPa	a (eV e	e ⁻¹)							2.2	0.0	10.0	13.4	10.7	24.4
3	Na ^{3s1}	Mg 3s ²	6 eV	e ⁻¹ ≈ 1	Paulin	ng unit							AI 3s ² 3p ¹	Si ^{3s²3p²}	P 3s ² 3p ³	S 3s ² 3p ⁴	CI 3s ² 3p ⁵	Ar 3s²3p ⁶
	-3.3	-2.3	3	4	5	6	7	8	9	10	11	12	-1.6	0.6	3.8	5.8	9.3	13.3
4	K ^{3d1} -8.5	Ca ^{3d²} -11.5	Sc ^{3d³} -14.0	Ti ^{3d⁴} -12.5	∨ _{3d⁵} -10.4	Cr ^{3d⁶} -7.5	Mn ^{3d7} -7.7	Fe ^{3d®} -9.5	Со ^{здэ} -7.5	Ni ^{3d¹⁰} -7.1	Cu ^{4s¹3d¹⁰} 2.7	Zn ^{4s²3d¹⁰} <i>8.7</i>	Ga ^{4s²4p¹} 1.5	Ge ^{4s²4p²} 2.5	As 4s ² 4p ³ 4.1	Se ^{4s²4p⁴} 5.3	Br 4s ² 4p ⁵ 7.9	Kr ^{4s²4p⁶ 10.8}
	Dh			7	Nb				Dh	Dd	۸a			<u> </u>	<u> </u>			
5	4d ¹	4d ²	4d ³	4d ⁴	4d⁵	4d ⁶	4d ⁷	4d ⁸ -5.6	4d ⁹	4d ¹⁰	5s ¹ 4d ¹⁰	5s ² 4d ¹⁰	5s ² 5p ¹ 1 /	5s ² 5p ²	5s ^{25p³}	5s ² 5p ⁴	5s²5p⁵ 5 8	5s ² 5p ⁶
	0.0										7.0					0.5		0.0
6	5d ¹	5d ²	5d ³	HT 5d⁴	5d⁵	6s ¹ 5d ⁵	5d7	5d ⁸	 5d ⁹	5d ¹⁰	AU 6s ¹ 5d ¹⁰	6s ² 5d ¹⁰	6s ² 6p ¹	6s ² 6p ²	6s ² 6p ³	PO 6s ² 6p ⁴	AT 6s ² 6p ⁵	6s ² 6p ⁶
•	-6.4	-9.2	-6.4	-7.9	-7.4	-3.1	-5.1	-2.5	-3.1	-1.5	3.7	7.5	2.6	3.1	2.7	4.1	4.9	7.3
7	Fr ^{6d1} -5.3	Ra ^{6d²} -6.4																
		6	La 5d ³	Ce 5d ² 4f ²	Pr 5d ² 4f ³	Nd 5d ² 4f ⁴	Pm 5d ² 4f ⁵	5d ² 4f ⁶	Eu 5d ² 4f ⁷	Gd 5d ³ 4f ⁷	TD 5d ³ 4f ⁸	Dy 5d ² 4f ¹⁰	HO 5d ³ 4f ¹⁰	Er 5d ² 4f ¹²	5d ² 4f ¹³	Yb 5d ² 4f ¹⁴		ement
			-9.8	-11.7	-7.2	-7.2	-6.8	-5.5	-4.2	0.8	1.3	-5.0	0.8	-5.8	-4.8	-2.1	atom con	figuration
		_	Ac		Pa			Pu	Am	Cm							@ 300) GPa
		7	6d ³		6d ³ 5f ²			6d ¹ 5f ⁷	6d ² 5f ⁷	6d ² 5f ⁸							2	
			-0. U		-10.0			-9.2	-4.1	-5.5								

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





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.



Model Validation of vdW radii (against noble gas elements)





38

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









- Relative size ordering can change
- There is something funny going on with Li...



H, Li, Na, K



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Alkaline Earth Atoms







What is 0.1Å worth?





The (Heavy) Main Group

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











The changes can be dramatic

Radius of Fe relative to Si







The changes can be dramatic









Or not very dramatic at all..

Radius of C relative to H





1.56

1.49 Francium

1 H	The vdW radii @ 300 GPa, Å 0.8 Å 0.8 Å																² He
0.85 Hydrogen										0.8 Å							0.81 Helium
^з Li 1.10	4 Be 1.18			R								₅ B 1.15	6 C 1.11	7 N 1.06	8 O 1.03	9 F 0.99	¹⁰ Ne 0.96
Lithium	Beryllium											Boron	Carbon	Nitrogen	Oxygen	Fluorine	Neon
Na	Mg											AI	Si	P	S	CI	Ar
1.18 Sodium	1.27 Magnesium									1.6 A		1.32 Aluminum	1.30 Silicon	1.28 Phosphorus	1.26 Sulfur	1.23 Chlorine	1.19 Argon
19	20	21 S c	22	23	24	25	26	27	28	29	30 7 m	31	32	33	34	35 D r	36
N 1.23 Potassium	Ca 1.28 Calcium	SC 1.21 Scandium	1.20 Titanium	V 1.23 Vanadium	Cr 1.20 Chromium	IVIN 1.20 Manganese	Fe 1.20 Iron	CO 1.20 Cobalt	INI 1.17 Nickel	Cu 1.23 _{Copper}	2.11 1.25 Zinc	Ga 1.29 Gallium	Ge 1.32 Germanium	AS 1.31 Arsenic	Se 1.31 Selenium	Dr 1.29 Bromine	Nr 1.27 Krypton
37 Dh	38 Sr	39 V	40 7 r	41	42 Mo	43 To	44 D 11	45 Dh	46 Dd	47	48 Cd	49	50 Sn	51 Sh	52 To	53	54
1.32 Rubidium	1.35 Strontium	1.34 Yttrium	LI 1.33 Zirconium	1.33 Niobium	1.31 Molybdenum	1.30 Technetium	nu 1.27 Ruthenium	1.25 Rhodium	1.24 Palladium	Ag 1.30 Silver	1.33 Cadmium	1.38 Indium	311 1.39 ™	1.40 Antimony	1.40 Tellurium	1.40 Iodine	1.39 Xenon
55 Ce	56 B 2		72 Hf	73 Ta	74 W	75 Bo	76	77 Ir	78 Dt	79 A 11	80 Ha	81 T I	82 Dh	83 Bi	84 P O	85	86 Bn
1.43 Cesium	Da 1.46 Barium		1.35 Hafnium	1.34 Tantalum	1.39 Tungsten	1.35 Rhenium	03 1.34 Osmium	1.32 Iridium	1.30 Platinum	1.32 Gold	1.33 Mercury	1.40 Thallium	1.42	1.42 Bismuth	1.43 Polonium	AL 1.44 Astatine	1.43 Radon
87 Fr	88 Ra																

X

0

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

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2.92 Radium

2.58 Francium

1 H 1.54	The vdW radii @ 1atm GPa, Å 1.3 Å														2 He 1. 34		
Hydrogen 3 Li 2.20 Lithium	4 Be 2.19 _{Beryllium}									1.3 A		5 B 2.05 Boron	6 C 1.90 _{Carbon}	7 N 1.79 Nitrogen	8 0 1.71 _{Oxygen}	9 F 1.63 Fluorine	Helium 10 Ne 1.56 Neon
11 Na 2.25 Sodium	12 Mg 2.40 _{Magnesium}			No.	All and					BoronCarbonNitrogenOxygenFluorine1314151617AISiPSCI2.392.322.322.232.142.06AluminumSiliconPhosphorusSulfurChlorine							
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 2.38 lodine	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 TI 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	88 Ra																

X

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



The Atoms Under Pressure Database

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

- radii

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- electronegativity
- electron configuration
- spin

Between 0 to 300 GPa!



	Elect	ronegativi	ty		Relative electronegativity vdW/non-bonded radii Spin													
Elect	roneg	jativit	y (eV	e ⁻¹) at	t P = 2	0 GP	а											
1 H 12.67 Hydrogen																	2 He 24.11 Helium	\$ @
3 Li 3.02 Lithium	4 Be 7.47 Beryllium											5 B 9.90 Boron	6 C 12.79 _{Carbon}	7 N 15.94 Nitrogen	8 0 17.78 _{Oxygen}	9 F 22.59 Fluorine	10 Ne 27.72 Neon	-
11 Na 3.07 Sodium	12 Mg 5.46 Magnesium											13 AI 6.96 Aluminum	14 Si 9.01 Silicon	15 P 11.25 Phosphorus	16 S 12.38 Sulfur	17 CI 15.20 Chlorine	18 Ar 18.24 Argon	
19 K 2.46 Potassium	20 Ca 3.64 _{Calcium}	21 SC 1.03 Scandium	22 Ti 2.27 Titanium	23 V 3.55 Vanadium	24 Cr 6.25 Chromium	25 Mn 6.26 _{Manganese}	30 Zn 14.53 _{Zinc}	31 Ga 8.12 Gallium	32 Ge 9.38 Germanium	33 As 10.97 Arsenic	34 Se 11.87 Selenium	35 Br 14.04 Bromine	36 Кг 16.34 _{Кгуртол}					
37 Rb 2.37 Bubidium	38 Sr 3.19 Strontium	39 Y 3.95 Yttrium	40 Zr 2.78 Zirconium	41 Nb 5.03 Nicolum	42 Mo 6.58 Molybdenum	43 TC 9.21 Technetium	44 Ru 6.82 Buthenium	48 Cd 14.69 _{Cadmium}	49 In 7.55 Indium	50 Sn 8.52 Tin	51 Sb 9.62 Antimony	52 Te 10.52 Tellurium	53 12.06	54 Xe 13.81 Xenon				
55 Cs 2.15 _{Cesium}	56 Ba -0.87 _{Barium}	La	72 Hf 5.02 Hafnium	73 Ta 5.95 Tantalum	74 W 4.49 Tungsten	75 Re 7.51 Rhenium	76 Os 7.63 _{Osmium}	80 Hg 12.97 Mercury	81 TI 8.59 Thallium	82 Pb 9.29 Lead	83 Bi 9.08 Bismuth	84 Po 10.65 Potonium	85 At 11.21 _{Astatine}	86 Rn 13.32 _{Radon}				
87 Fr 2.32 Francium	88 Ra 2.94 Radium	Ac																
			57 La -0.38	58 Ce 1.60 _{Cerium}	59 Pr 2.55 Praseodymium	60 Nd 3.00 Neodymium	61 Pm 5.08 Promethium	62 Sm 6.11 _{Samarium}	63 Eu 7.20 Europium	64 Gd 9.62 Gedolinium	65 Tb 5.53 Terbium	66 Dy 6.21 _{Dysprosium}	67 HO 6.28 Holmium	68 Er 5.51 Erbium	69 Tm 6.89 Thulium	70 Yb 8.17 Ytterbium	71 Lu 4.14	
	Corrum Praseodymium Neodymium Promethium Samarium Filledolum Samarium Filledolum 89 90 91 92 93 94 95 96 Acc Th Pa U - 5.25 6.27 8.88 2.12 - Protectinium Function - - -																	
Pressure	(GPa): 2	0																
		S	eparate co	olor scales	s for each p	oressure						One	color scale	o for all pre	ssures			
Select rel	ect relative plotting:																	
								Downloa	d selected	data								





Relating Chemical Concepts Using Pressure (a teaser)

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Relating atomic energy, radius and electronegativity through compression

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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 <u>non-bonded</u> 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)

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

Questions?

