

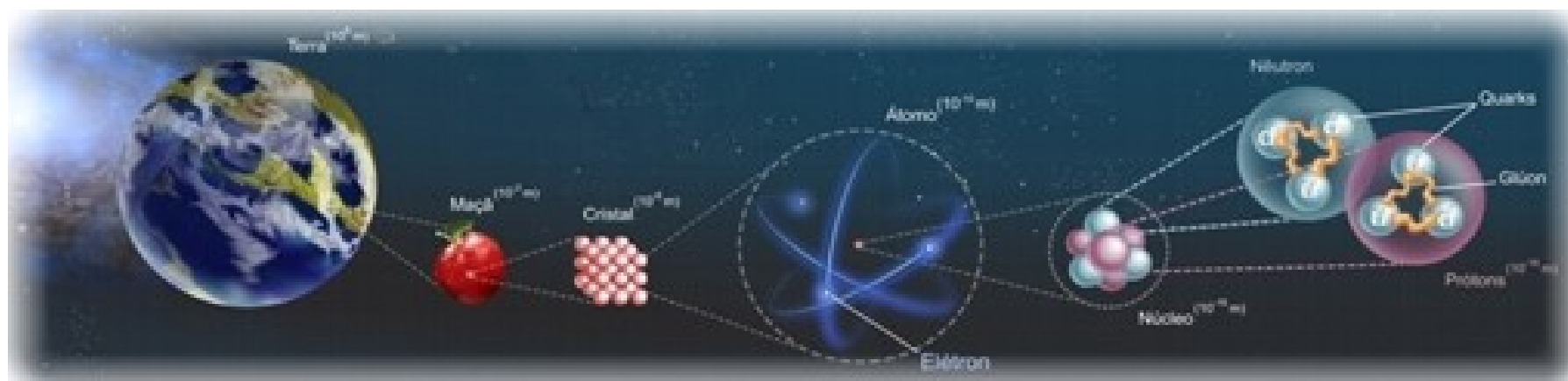


# **Estrutura da Matéria**

## **2018-2 – Prof. Célio**

### **Aula 7 – Orbitais atômicos e**

### **Tabela periódica (cont.)**

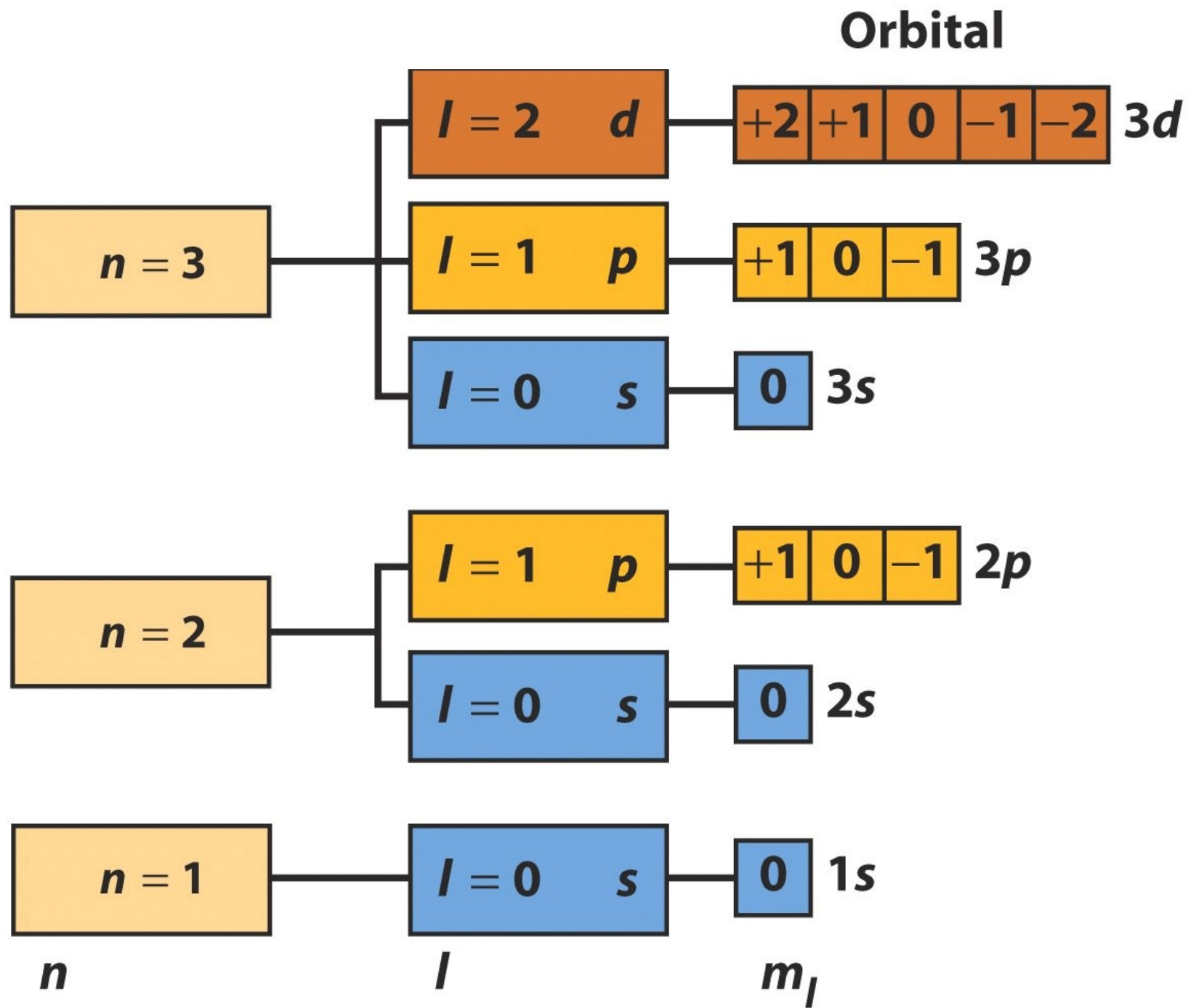


# Tabela com os números quânticos para elétrons nos átomos

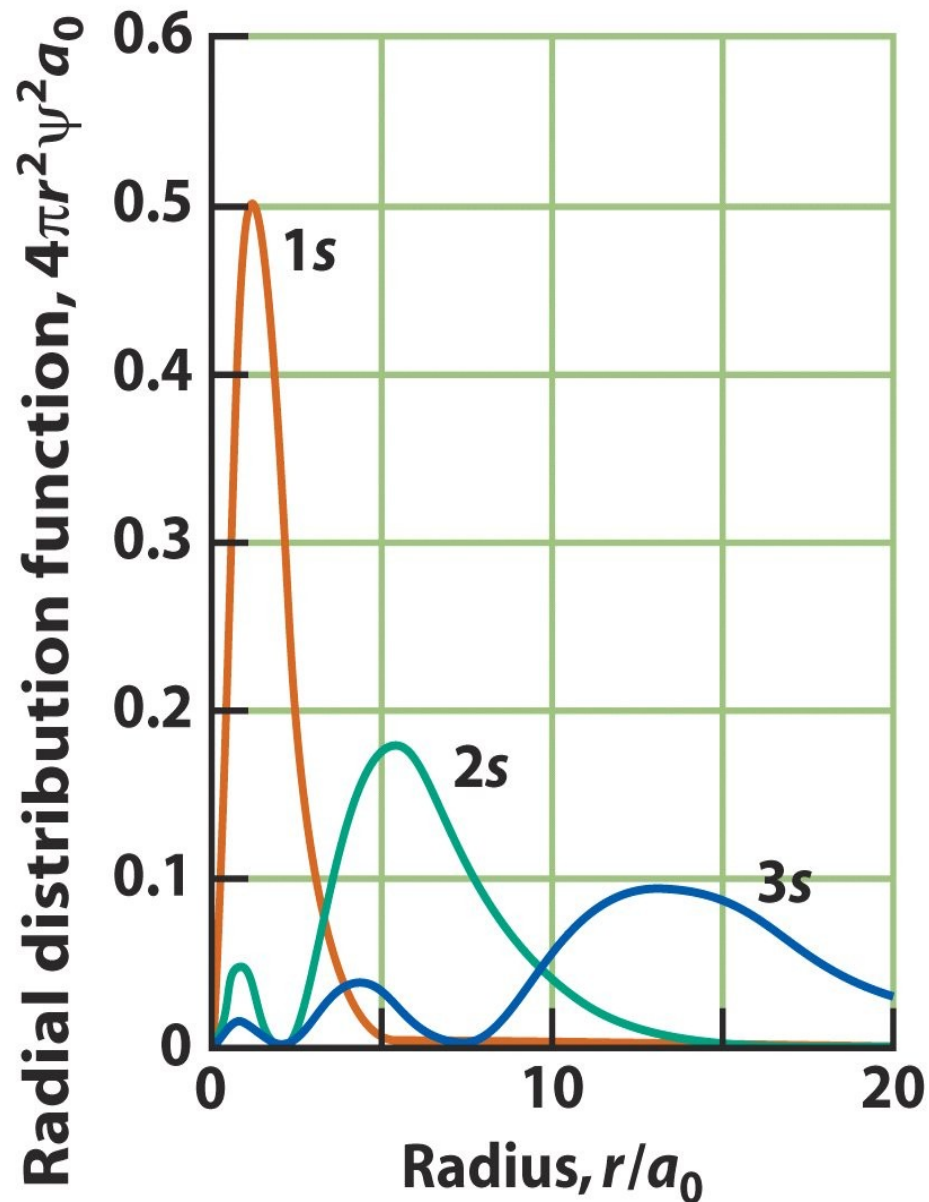
**TABLE 1.3** Quantum Numbers for Electrons in Atoms

Name	Symbol	Values	Specifies	Indicates
principal	$n$	$1, 2, \dots$	shell	size
orbital angular momentum*	$l$	$0, 1, \dots, n - 1$	subshell: $l = 0, 1, 2, 3, 4, \dots$ $s, p, d, f, g, \dots$	shape
magnetic	$m_l$	$l, l - 1, \dots, -l$	orbitals of subshell	orientation
spin magnetic	$m_s$	$+\frac{1}{2}, -\frac{1}{2}$	spin state	spin direction

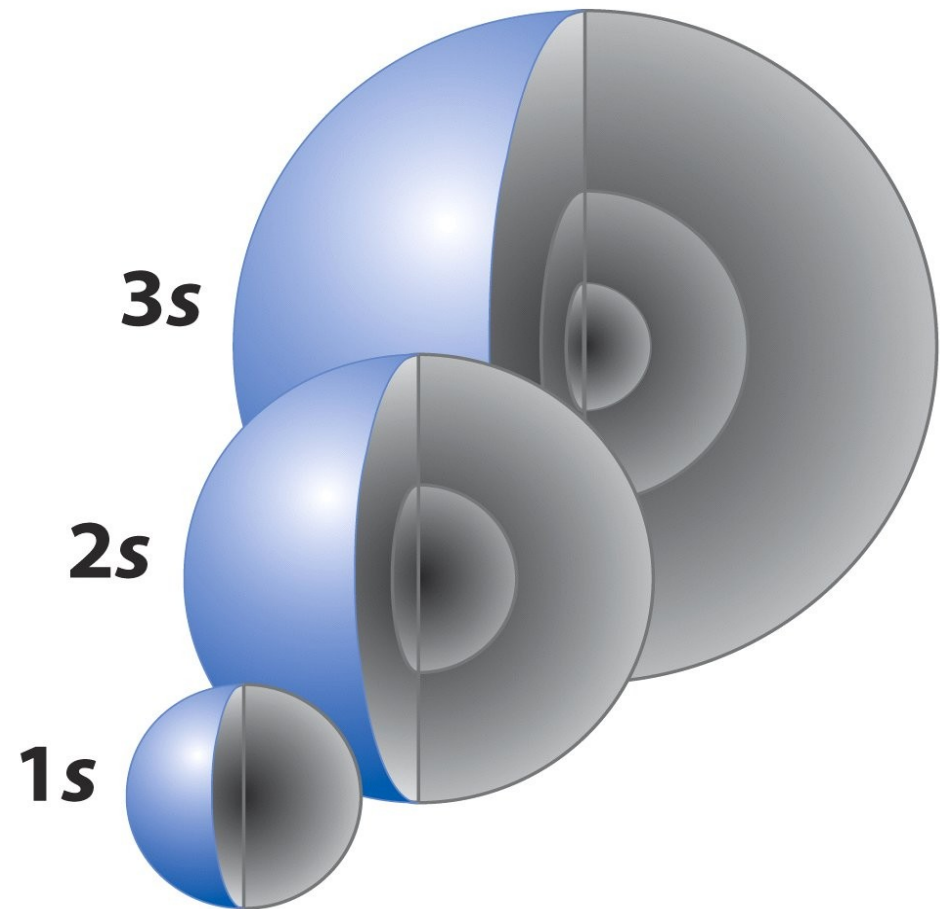
\*Also called the *azimuthal quantum number*.



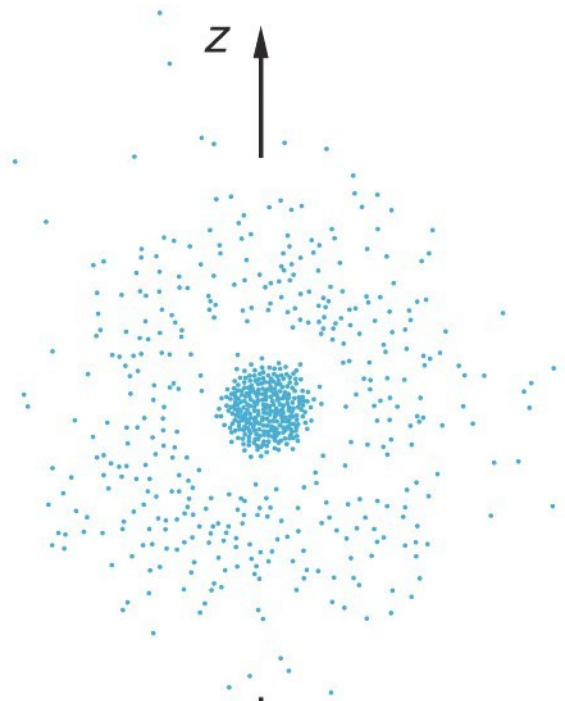
# Função de Distribuição Radial



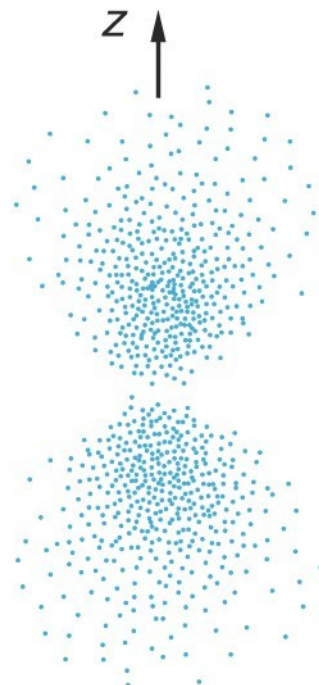
Aparência em 3 dimensões  
dos orbitais s



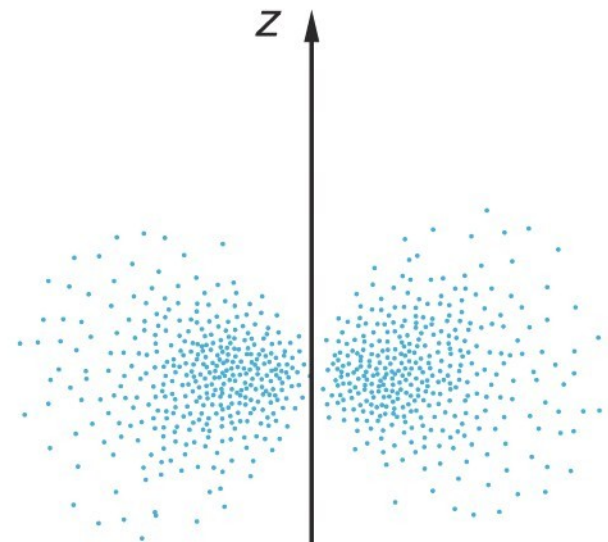
# Densidades de probabilidade para $n=2$



$n = 2$   
 $l = 0$   
 $m = 0$



$n = 2$   
 $l = 1$   
 $m = 0$



$n = 2$   
 $l = 1$   
 $m = \pm 1$

# Átomos com muitos elétrons:

## Preenchimento dos orbitais atômicos

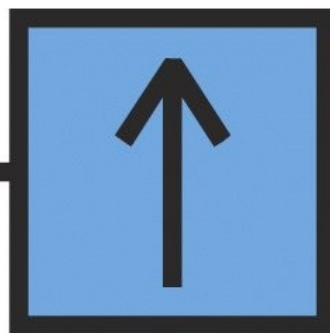
- Dados  $N$  elétrons, como eles se distribuem no átomo?

$n$					
1	$K$	$s^2$			
2	$L$	$s^2$	$p^6$		
3	$M$	$s^2$	$p^6$	$d^{10}$	
4	$N$	$s^2$	$p^6$	$d^{10}$	$f^{14}$
5	$O$	$s^2$	$p^6$	$d^{10}$	$f^{14}$
6	$P$	$s^2$	$p^6$	$d^{10}$	
7	$Q$	$s^2$			

# Princípio da construção

- Adicione elétrons, um após o outro, aos orbitais, na ordem da figura seguinte, porém não coloque mais de dois elétrons por orbital. → Princípio da exclusão de Pauli
- Se mais de um orbital em uma camada estiver disponível, adicione elétrons com spins paralelos aos diferentes orbitais daquela subcamada até completá-la, antes de emparelhar dois elétrons em um dos orbitais. → Regra de Hund

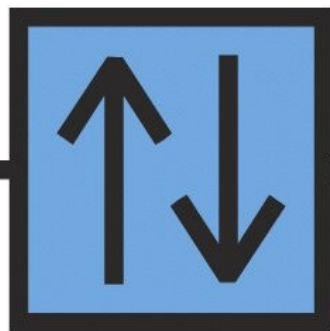
**1s**



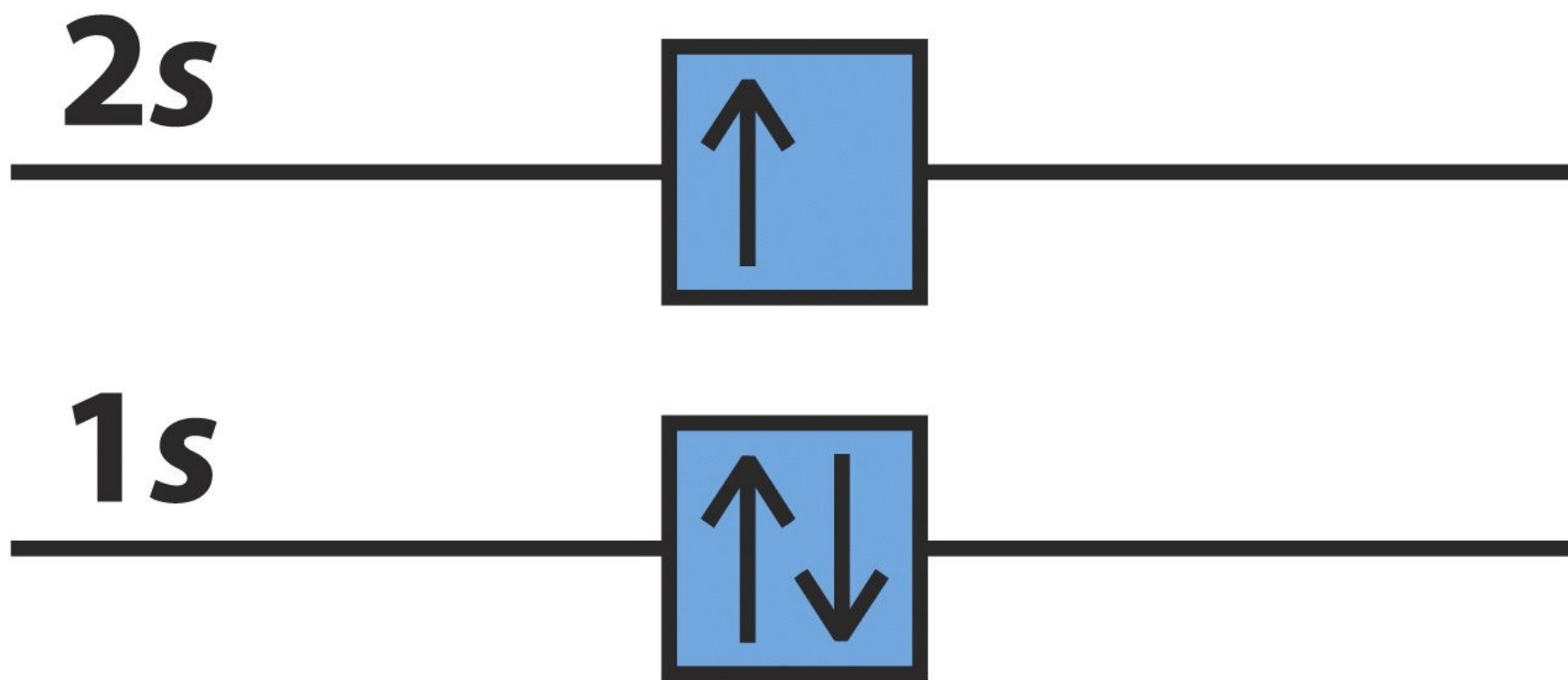
**1 H 1s<sup>1</sup>**



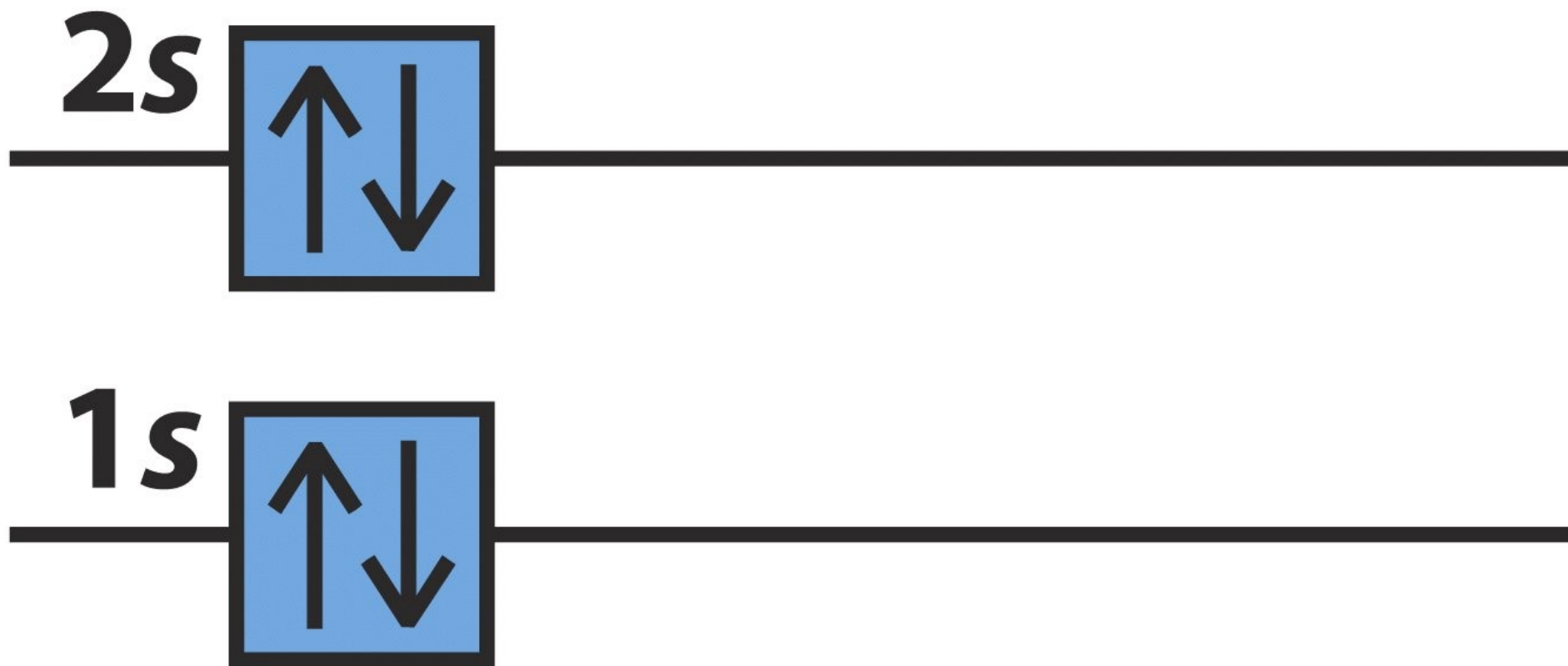
**1s**



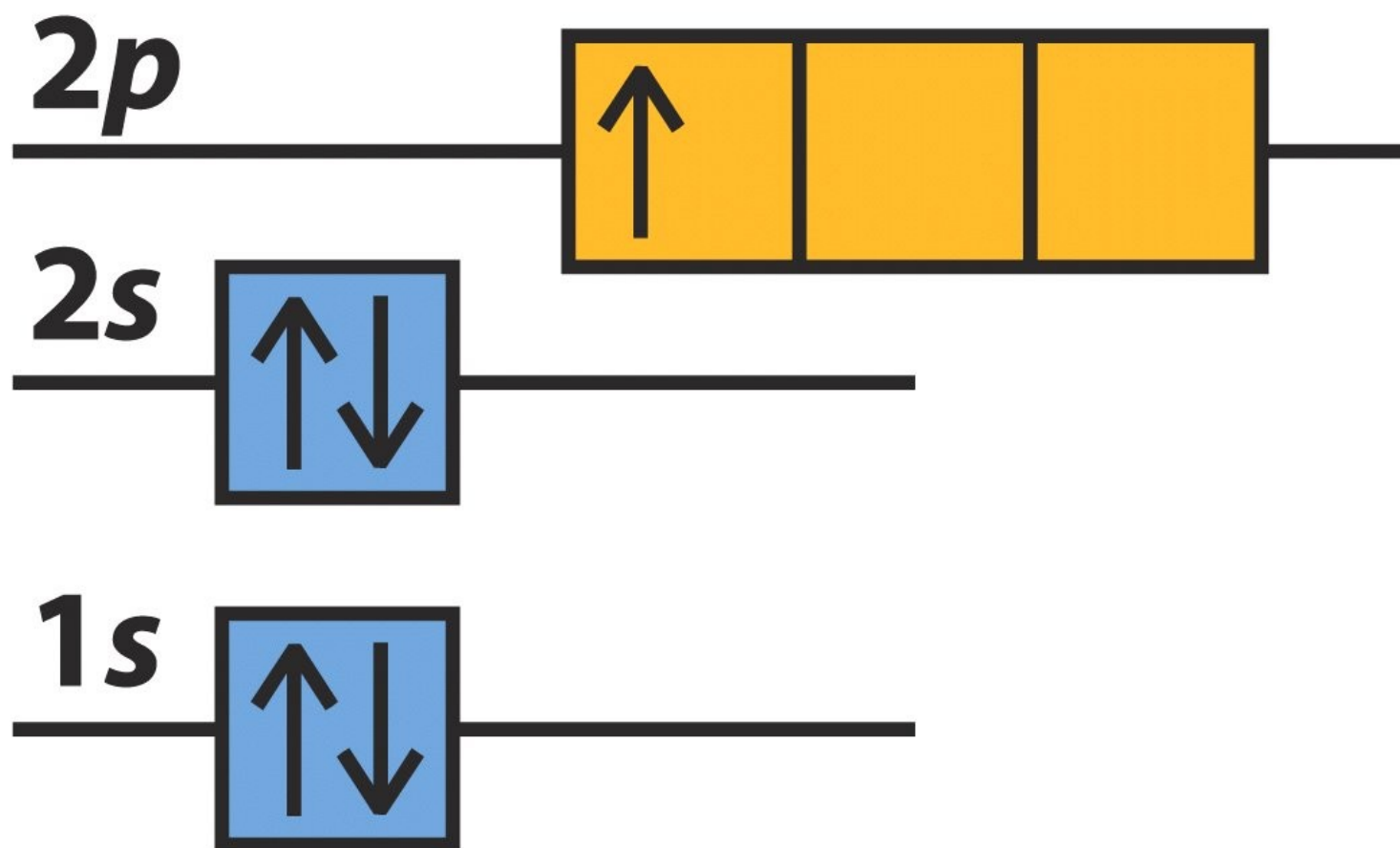
**2 He 1s<sup>2</sup>**



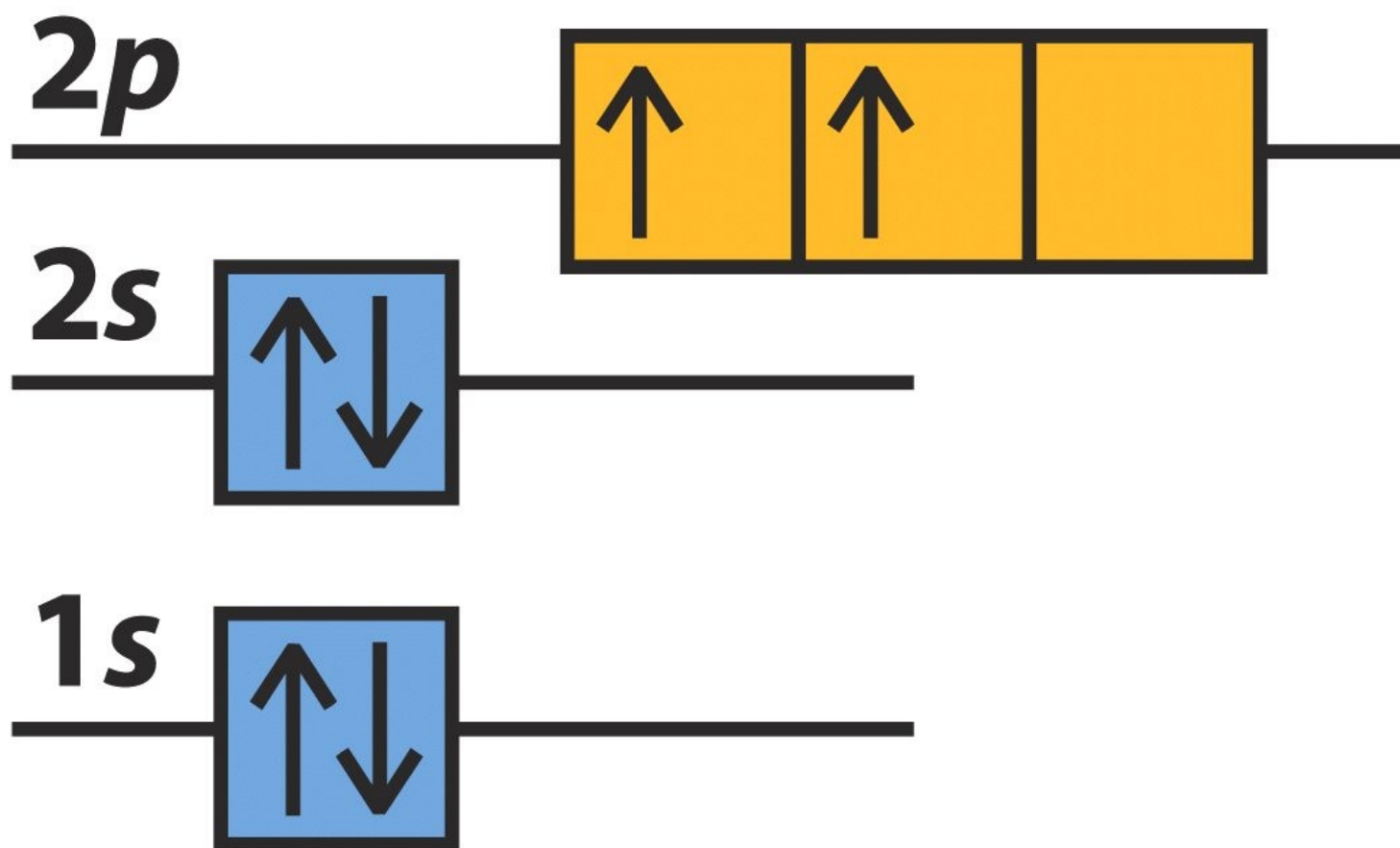
**3**    **Li  $1s^2 2s^1$ , [He] $2s^1$**



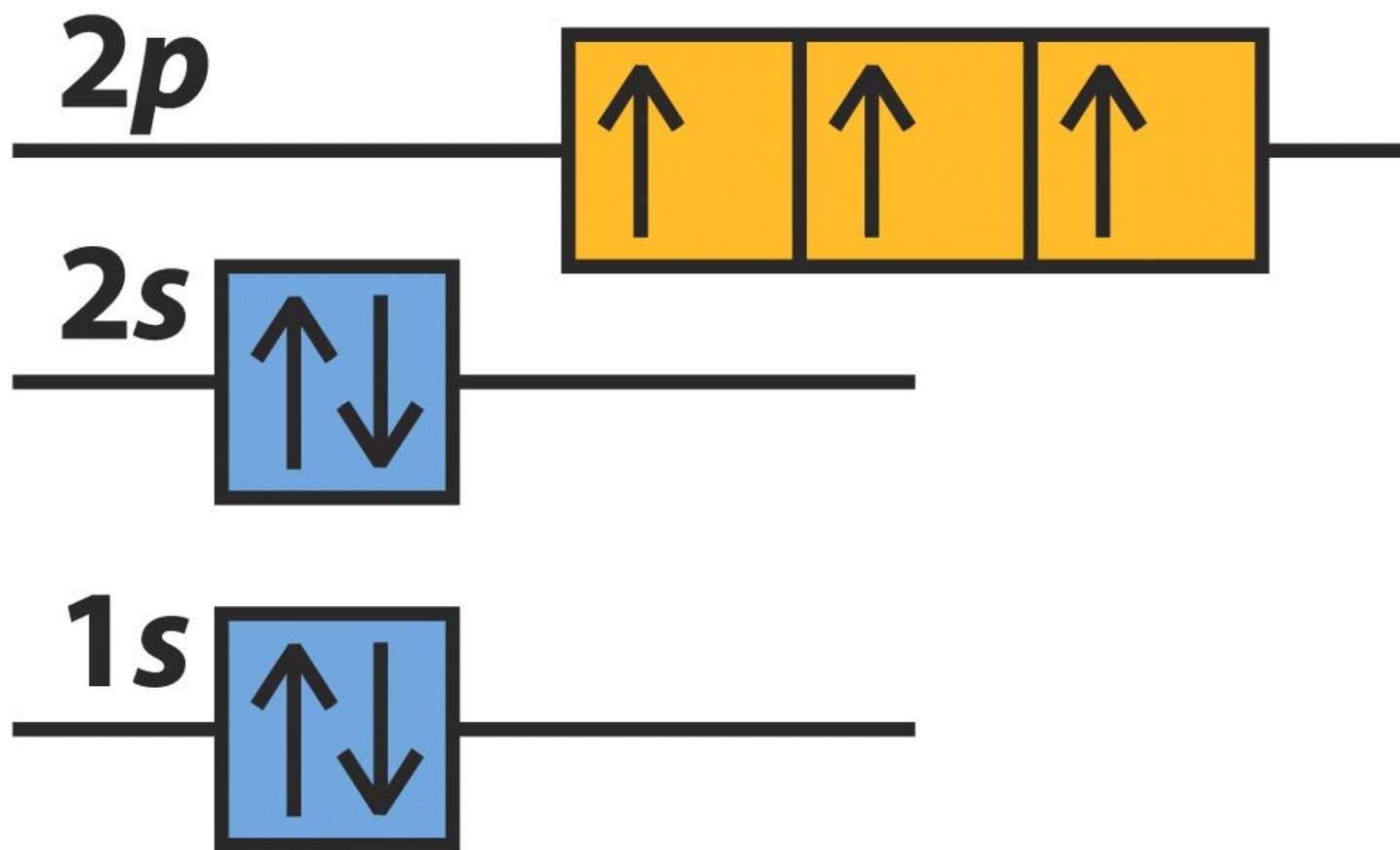
**4**     **Be  $1s^2 2s^2$ , [He]  $2s^2$**



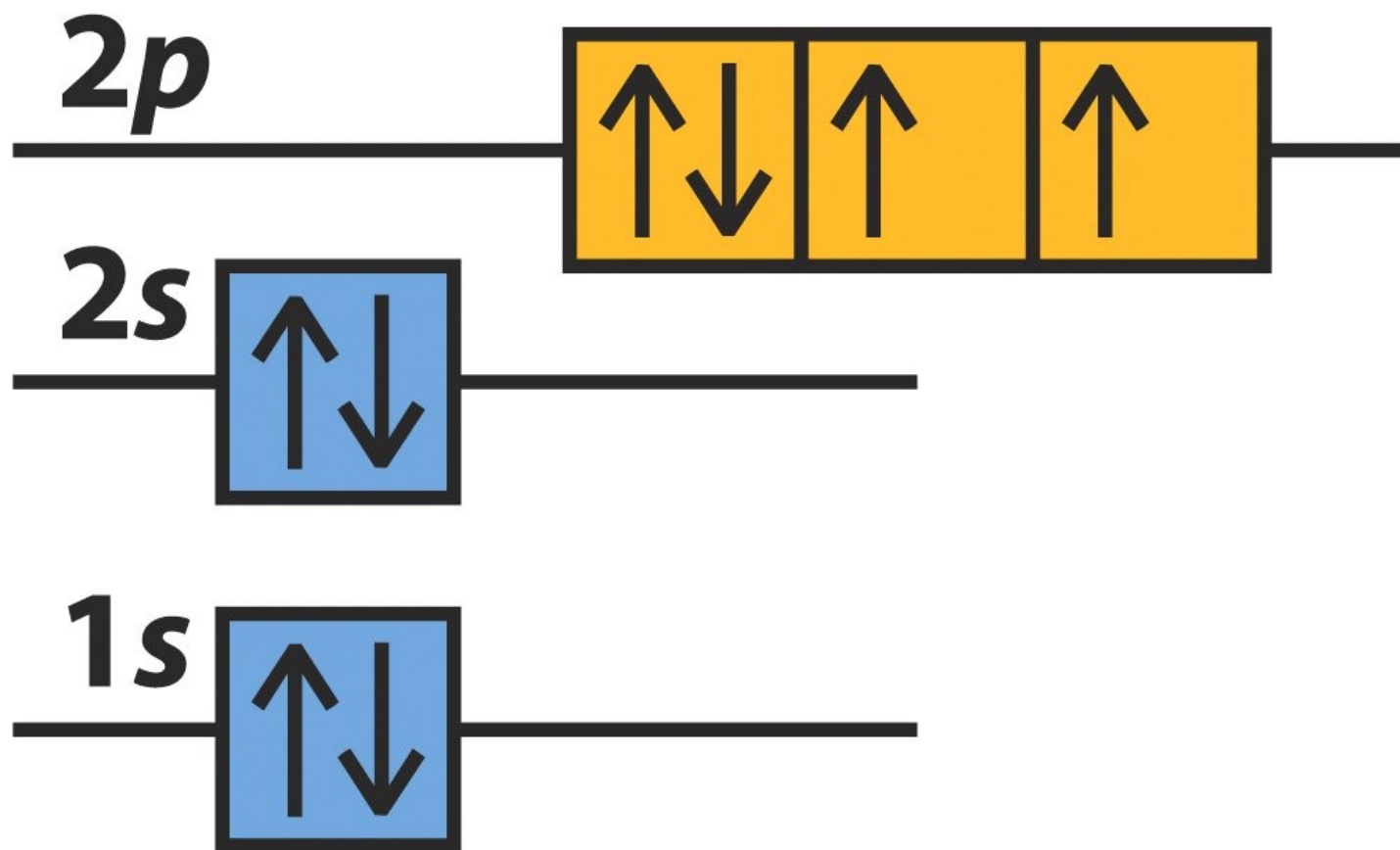
**5 B  $1s^2 2s^2 2p^1$ , [He]  $2s^2 2p^1$**



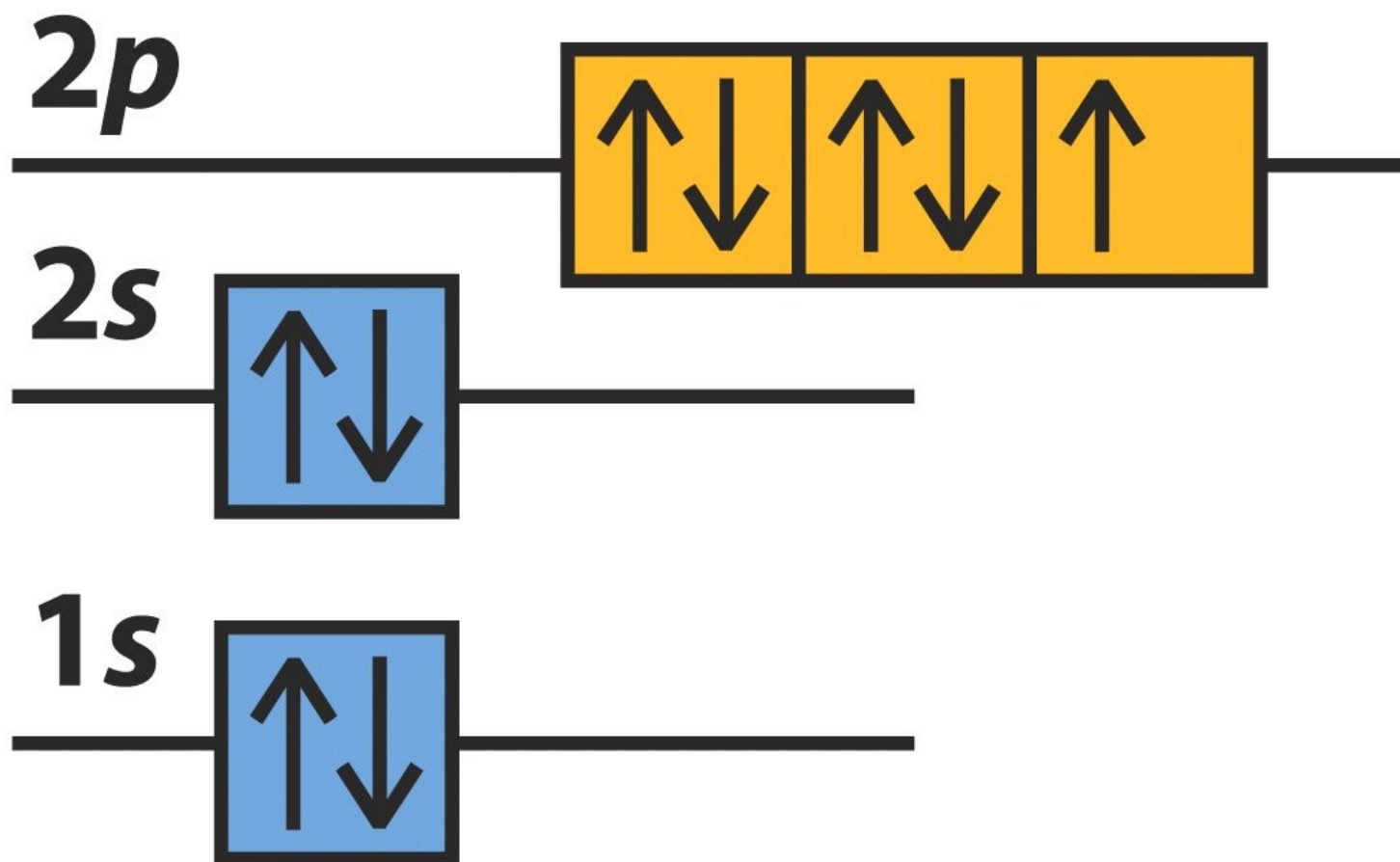
**6 C  $1s^2 2s^2 2p^2$ , [He]  $2s^2 2p^2$**



**7**     **N**  $1s^2 2s^2 2p^3$ , **[He]**  $2s^2 2p^3$

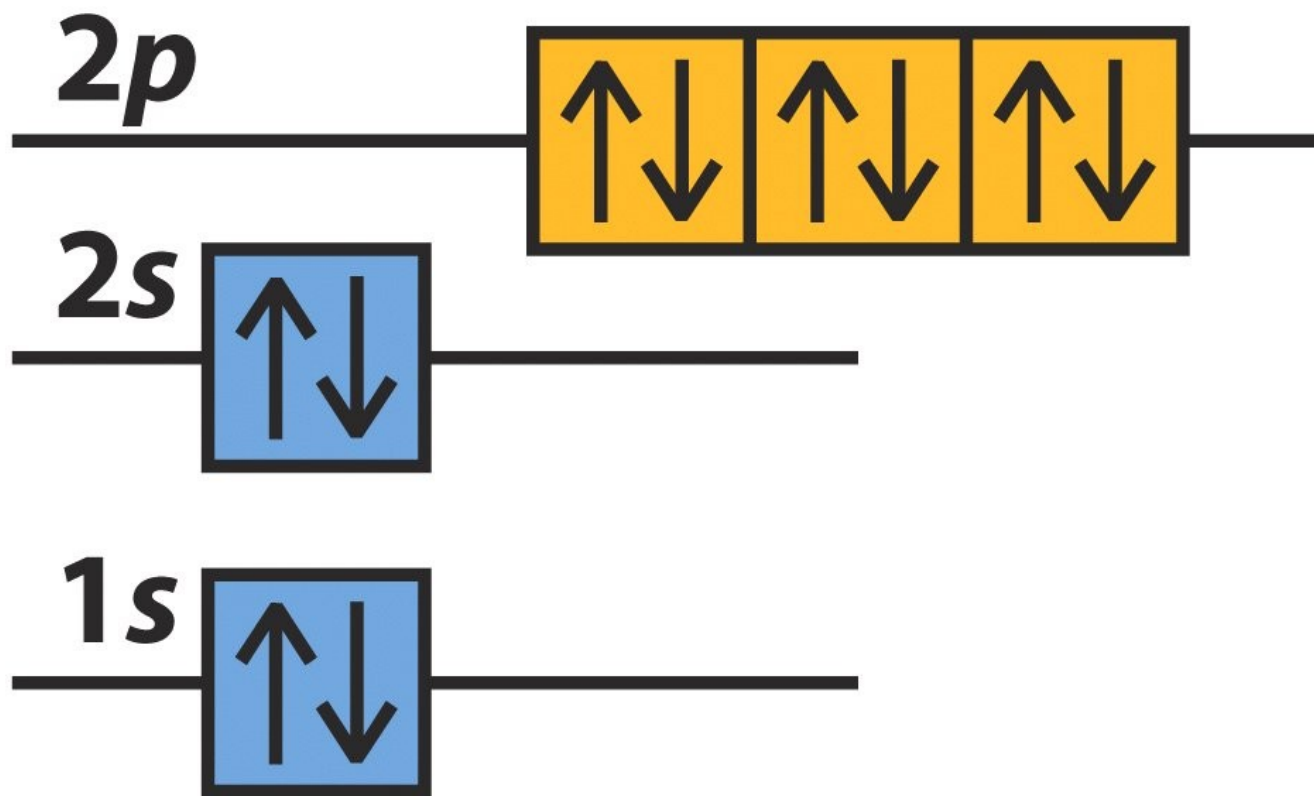


**8      0  $1s^2 2s^2 2p^4$ , [He]  $2s^2 2p^4$**

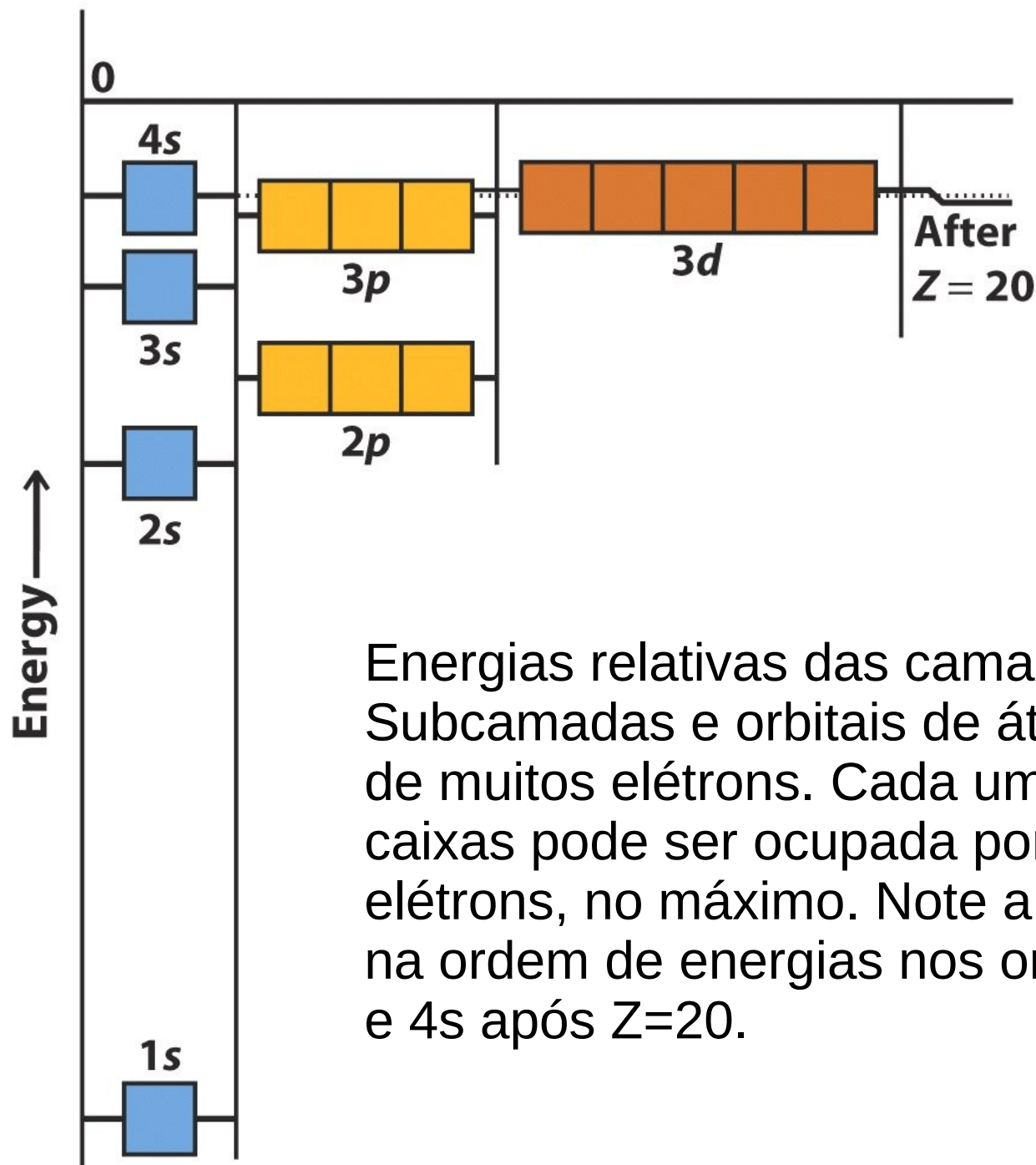


**9 F  $1s^2 2s^2 2p^5$ , [He]  $2s^2 2p^5$**



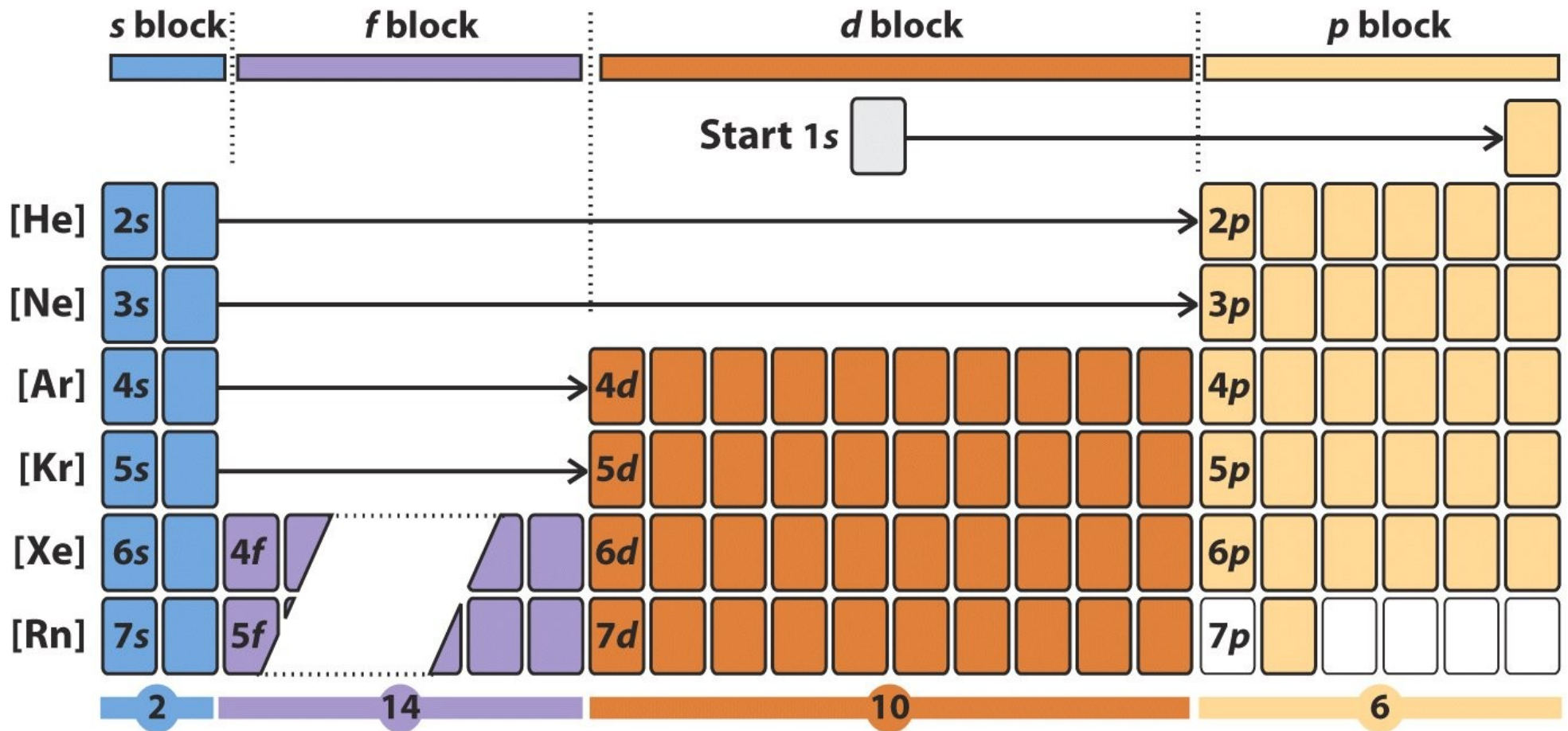


**10      Ne  $1s^2 2s^2 2p^6$ , [He]  $2s^2 2p^6$**



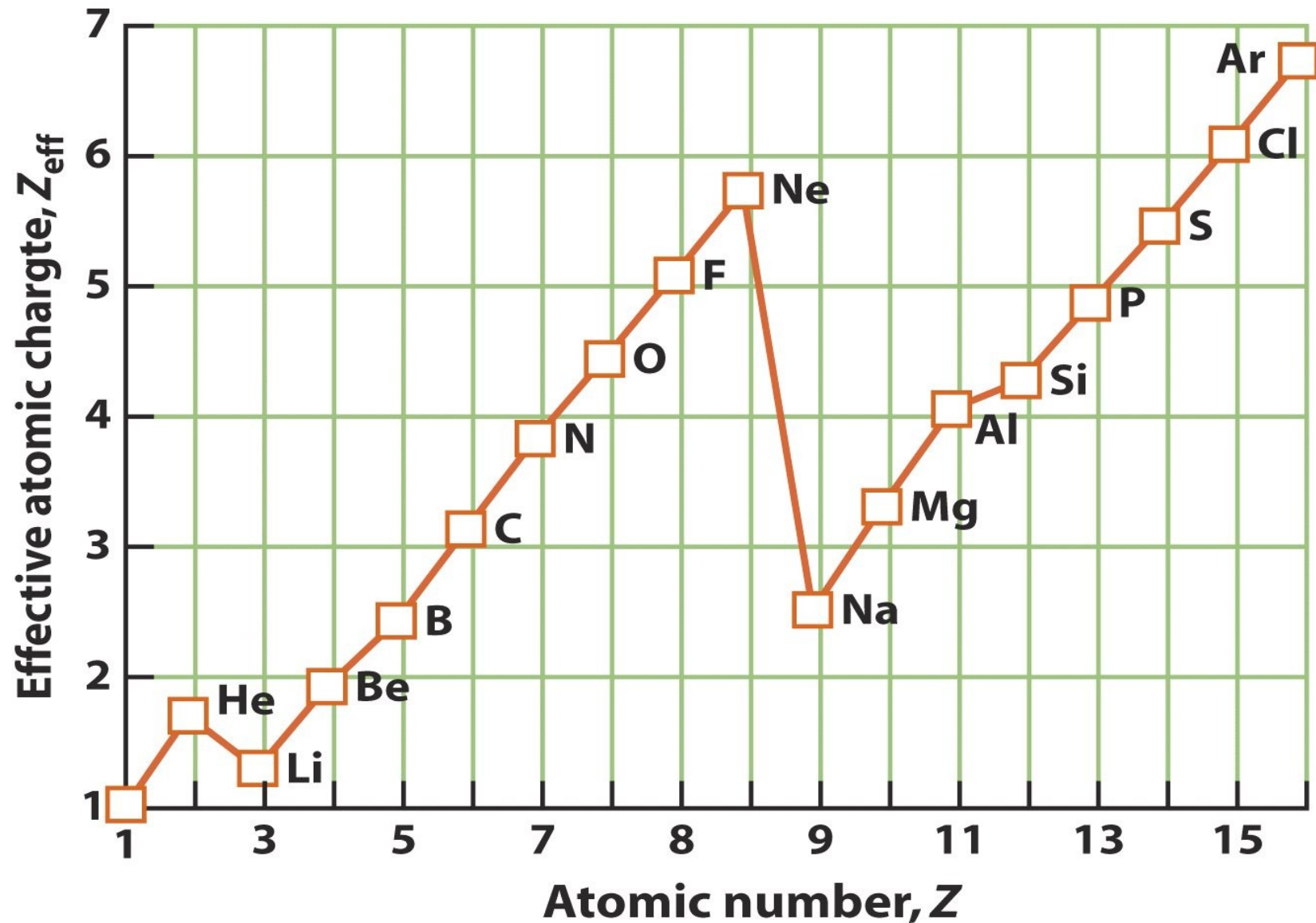
Energias relativas das camadas, Subcamadas e orbitais de átomos de muitos elétrons. Cada uma das caixas pode ser ocupada por dois elétrons, no máximo. Note a mudança na ordem de energias nos orbitais 3d e 4s após  $Z=20$ .

# Tabela Periódica

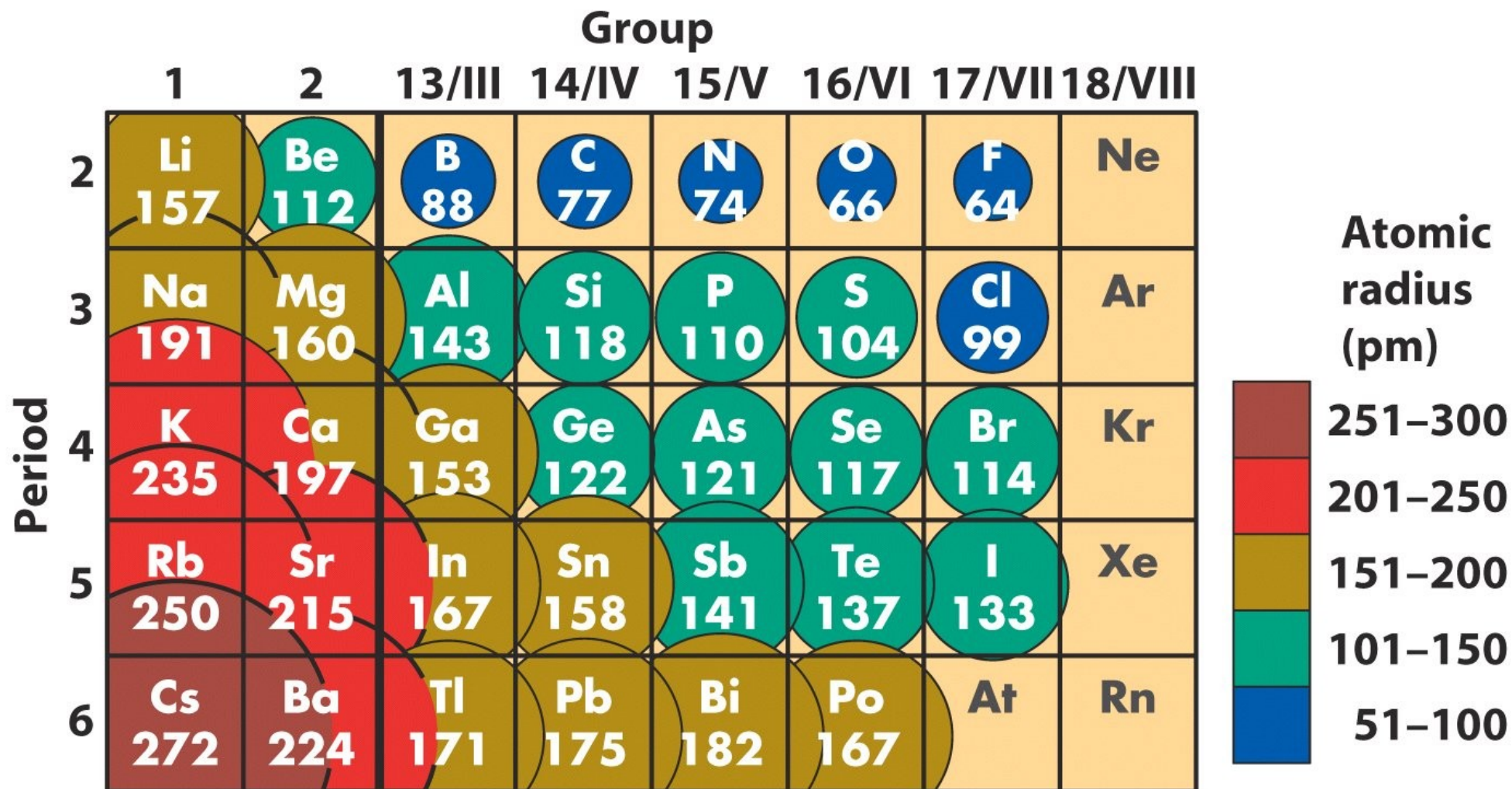


# Propriedades periódicas

## Carga Efetiva



# Propriedades Periódicas





# Propriedades Periódicas

		Group							
		1	2	13/III	14/IV	15/V	16/VI	17/VII	18/VIII
Period	2	Li 58	Be <sup>2+</sup> 27	B <sup>3+</sup> 12	C	N <sup>3-</sup> 171	O <sup>2-</sup> 140	F <sup>-</sup> 133	Ne
	3	Na <sup>+</sup> 102	Mg <sup>2+</sup> 72	Al <sup>3+</sup> 53	Si	P <sup>3-</sup> 212	S <sup>2-</sup> 184	Cl <sup>-</sup> 181	Ar
	4	K <sup>+</sup> 138	Ca <sup>2+</sup> 100	Ga <sup>3+</sup> 62	Ge	As <sup>3-</sup> 222	Se <sup>2-</sup> 198	Br <sup>-</sup> 196	Kr
	5	Rb <sup>+</sup> 149	Sr <sup>2+</sup> 116	In <sup>3+</sup> 72	Sn	Sb	Te <sup>2-</sup> 221	I <sup>-</sup> 220	Xe
	6	Cs <sup>+</sup> 170	Ba <sup>2+</sup> 136	Tl <sup>3+</sup> 88	Pb	Bi	Po	At	Rn

Ionic radius (pm)

- 201–250
- 151–200
- 101–150
- 51–100
- 1–50

# Propriedades Periódicas

## Energia de ionização

		Group						18/VIII	
		1	2	13/III	14/IV	15/V	16/VI	17/VII	
Period									<div>H 1310</div>
	2	<div>Li 519</div>	<div>Be 900</div>	<div>B 799</div>	<div>C 1090</div>	<div>N 1400</div>	<div>O 1310</div>	<div>F 1680</div>	<div>He 2370</div>
	3	<div>Na 494</div>	<div>Mg 736</div>	<div>Al 577</div>	<div>Si 786</div>	<div>P 1011</div>	<div>S 1000</div>	<div>Cl 1255</div>	<div>Ar 1520</div>
	4	<div>K 418</div>	<div>Ca 590</div>	<div>Ga 577</div>	<div>Ge 784</div>	<div>As 947</div>	<div>Se 941</div>	<div>Br 1140</div>	<div>Kr 1350</div>
	5	<div>Rb 402</div>	<div>Sr 548</div>	<div>In 556</div>	<div>Sn 707</div>	<div>Sb 834</div>	<div>Te 870</div>	<div>I 1008</div>	<div>Xe 1170</div>
	6	<div>Cs 376</div>	<div>Ba 502</div>	<div>Tl 590</div>	<div>Pb 716</div>	<div>Bi 703</div>	<div>Po 812</div>	<div>At 1037</div>	<div>Rn 1036</div>

Ionization energy (kJ·mol<sup>-1</sup>)

2001–2500

1501–2000

1001–1500

501–1000

1–500

# Propriedades Periódicas

## Afinidade eletrônica

		Group						18/VIII	
		1	2	13/III	14/IV	15/V	16/VI	17/VII	
Period	2	Li +60	Be ≤0	B +27	C +122	N -7	O +141 -844	F +328	Ne ≤0
	3	Na +53	Mg ≤0	Al +43	Si +134	P +72	S +200 -532	Cl +349	Ar ≤0
	4	K +48	Ca +2	Ga +29	Ge +116	As +78	Se +195	Br +325	Kr ≤0
	5	Rb +47	Sr +5	In +29	Sn +116	Sb +103	Te +190	I +295	Xe ≤0
	6	Cs +46	Ba +14	Tl +19	Pb +35	Bi +91	Po +174	At +270	Rn ≤0

Electron affinity (kJ·mol<sup>-1</sup>)

- >300
- 200–300
- 100–200
- 0–100
- <0



# Bibliografia

- Atkins e Jones, Princípios de Química, cap. 1, ed. Bookman (2012).