Quantum Mechanics

- Quantum Numbers
  - Pauli Exclusion Principle
  - Aufbau Principle
  - Hund's Rule
  - Valence Electrons

- Periodic Table Trends
  - Ionization Energy
  - Electron Affinity
  - Atomic Radii

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Pauli Exclusion Principle

In an atom, no two $e^-$ can have the same set of quantum #'s.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$l$</th>
<th>Orbital Designation</th>
<th>$m_l$</th>
<th>Number of Orbitals</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>$1s$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>$2s$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$2p$</td>
<td>$-1, 0, +1$</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>$3s$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$3p$</td>
<td>$-1, 0, 1$</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>$4s$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$4p$</td>
<td>$-1, 0, 1$</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>$5s$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$5p$</td>
<td>$-1, 0, 1$</td>
<td>3</td>
</tr>
</tbody>
</table>

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Aufbau Principle

Electrons add one by one to atomic orbitals to “build up” from lower to higher energy states.

Each orbital can hold 2 $e^-$. 
Aufbau Principle

Electrons add one by one to atomic orbitals to "build up" from lower to higher energy states.

Only 2 e⁻ in the 2p subshell

"p" subshell can hold up to 6 e⁻

"s" subshell can hold only 2 e⁻

Hund’s Rule

When several orbitals are of equal energy, a single e⁻ enters each orbital before a second e⁻ enters.

C: 1s² 2s² 2pₓ¹ 2pᵧ¹

Hund’s Rule

The spin of electrons filling orbitals of the same energy level remain parallel until electron pairs can be formed.

N: 1s²2s²2pₓ¹2pᵧ¹2pₓ¹ utenberg

O: 1s²2s²2pₓ¹2pᵧ¹2pₓ¹ utenberg
Week 5  
CHEM 1310 - Sections L and M

Valence Electrons

- Electrons in the outermost (i.e. highest energy) shell of an atom
- Directly involved in bonding
- Number of valence e\(^{-}\) is same as the Group # in the Periodic Table

Increasing # of valence e\(^{-}\) across period

1s\(^2\) 2s\(^2\) 2p\(^x\)\(^{2}\) 2p\(^y\)\(^{1}\) 2p\(^z\)\(^{1}\)

# of e\(^{-}\) in the outermost shell 6

Notice that 2 of oxygen’s valence e\(^{-}\) are unpaired!
PRS Question
Who developed the theory that no two electrons can have the same set of quantum numbers?

(1) Hund
(2) Aufbau
(3) Heisenberg
(4) Pauli
(5) Einstein

Pauli Exclusion Principle
**PRS Question**

What is the maximum number of electrons that can occupy the orbitals with principle quantum number = 4?

- (1) 2
- (2) 8
- (3) 18
- (4) 32
- (5) None of the above

<table>
<thead>
<tr>
<th>n</th>
<th>l</th>
<th>Orbital Designation</th>
<th>4s</th>
<th>4p</th>
<th>4d</th>
<th>4f</th>
<th>Sum</th>
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<td>2</td>
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<td>1</td>
<td>4p</td>
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<td>2</td>
<td>4d</td>
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<td></td>
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<tr>
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<td>3</td>
<td>4f</td>
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<td></td>
<td>32</td>
</tr>
</tbody>
</table>

**PRS Question**

Which of the following elements has 4 valence electrons?

- (1) Be
- (2) Si
- (3) P
- (4) Al
- (5) As

**PRS Question**

Which of the following elements has 4 valence electrons?

- (1) Be - 2
- (2) Si
- (3) P - 5
- (4) Al - 3
- (5) As - 5
How many valence electrons does Mg$^{2+}$ have?

- (1) 0
- (2) 1
- (3) 2
- (4) 3
- (5) 12

Mg is in Group 2 (meaning 2 valence e$^-$) but Mg$^{2+}$ has lost them!

Ionization energy is that required to remove an e$^-$ from a gaseous atom or ion in the ground state.
Atomic Radius

The radius of an atom (\(r\)) is defined as half the distance between the nuclei in a molecule consisting of identical atoms.

\[
\frac{2r}{\text{Br}} \quad \frac{2r}{\text{Br}}
\]

Comparing Atomic Radii

Elements with very different \# of electron can have similar atomic radii.

<table>
<thead>
<tr>
<th>Na</th>
<th>Mg</th>
<th>Al</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cl</th>
<th>Ar</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>14</td>
<td>15</td>
<td>16</td>
<td>17</td>
<td>18</td>
<td>19</td>
<td>20</td>
</tr>
</tbody>
</table>

Distance in picometers: \(1 \times 10^{-12} \text{ m}\)

Periodic Trends: Atomic Radii

- Atomic radius increases down a group
- Atomic radius decreases across a period
Next Week

- Recap of Chapter 12
  - Summary of what to learn re: Quantum Mechanics
  - More practice questions re: QM

- Begin Chapter 13: Bonding
  - Read entire chapter