Mendeleev categorizes elements by similar chemical bondings, physical properties etc. and orders elements by *atomic weight*. (wrong)

i.e. all based on *macroscopic* properties.

Many missing elements, and the types of bonds (“properties”) get increasingly hard to describe for heavy elements.

However, there are two “holes” in the table that are discovered:

* germanium
* gallium

But no underlying theory (yet) as to why this pattern exists.....
The other problem with Bohr’s atom

The shells of the Bohr model were *postulated* to account for the quantized spectrum.

De Broglie’s waves explained the origin of quantization.

But in elements with many electrons why do the electrons go to higher energy orbits instead of all occupying the lowest energy orbit?

The solution:
- electrons have one more quantum number: spin
- Pauli exclusion principle

No two “fermions” can be in the *same state*.
(i.e. at least one of the “quantum numbers” must be different)
What are “fermions”? To answer this we need an additional quantum number spin.

Earth “spins” on its axis as it goes around the sun.

Other particles (electrons, protons, neutrons,...) also spin around their own axes.

Unlike large objects, the spin is quantized (can only take particular values). For electrons, protons and neutrons only two options called “spin up” and “spin down”
Bosons v. Fermions

Orbitals: \(2\ell + 1\) possible orientations \((m)\) values

Spin \(s\): \(2s + 1\) possible orientations \((m)\) values

Electrons have two orientations \(\Rightarrow \) “spin \(\frac{1}{2}\)”

Fermions are particles with an even number of possible orientations \((s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots)\)

Bosons are particles with an odd number of possible orientations \((s = 0, 1, 2, \ldots)\)

Bosons “want” to be in the same state.
(critical for lasers!)

Fermions \(\textit{cannot}\) to be in the same state.
This is the Pauli principle!
(critical for atomic structure!)

<table>
<thead>
<tr>
<th>Fermion</th>
<th>Boson</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrons</td>
<td>Photon</td>
</tr>
<tr>
<td>Neutron</td>
<td>He-3</td>
</tr>
<tr>
<td>Proton</td>
<td>He-4</td>
</tr>
<tr>
<td></td>
<td>:</td>
</tr>
<tr>
<td>Quarks</td>
<td>Gluons</td>
</tr>
<tr>
<td>Neutrino</td>
<td>W/Z bosons</td>
</tr>
</tbody>
</table>

Familiar particles
Atoms
Other elementary particles
Start by looking at the different possible states

<table>
<thead>
<tr>
<th>n</th>
<th>l</th>
<th>m</th>
<th>spin</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>Up</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>Down</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>Up</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>Down</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>-1</td>
<td>Up</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>-1</td>
<td>Down</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>Up</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>Down</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>Up</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>Down</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>Up</td>
</tr>
<tr>
<td>etc</td>
<td>etc</td>
<td>etc</td>
<td>etc</td>
</tr>
</tbody>
</table>

Two electrons to fill n=1 “shell”

Eight electrons to fill n=2 “shell”

Electron in n=2 shell cannot fall into the n=1 shell as all the states are already taken!
The energy level structure

For hydrogen, only the “n” quantum number was needed to get the energy.

In heavier elements, electron-electron interactions make energy depend on n and l.

For hydrogen, typical multi-electron atoms

\[ m \text{ and spin still } \sim \text{“degenerate”}, \text{ so not shown on this diagram} \]
The inert elements

Typical multi-electron atoms

Energy

- 1s
- 2s
- 2p
- 3s
- 3p
- 4s
- 4p
- 3d
- 10 states
- 6 states
- 2 states
- 6 states
- 2 states
- 2 states

Filling up the p shells is where the large gaps occur -- these are the inert elements!

Test yourself:
How many protons does the second (i.e. not Helium) inert (“noble”) gas have? You only need the diagram on the left.
Chemistry = Schroedinger energy levels + Pauli principle!

• Only the outer levels of the electrons useful for bonding
• Structure of table mimics the electron shell structure
  (Note that elements are characterized by *atomic number*,
  not *atomic weight* first proposed by Mendeleev)
Covalent bonding

Hydrogen-Hydrogen bonding

Wavefunctions squished -
Wavelength decreases –
$E=\frac{p^2}{2m} \sim \frac{1}{\lambda^2}$ –
Energy increases

Wavefunctions expand -
wavelength increases –
$E=\frac{p^2}{2m} \sim \frac{1}{\lambda^2}$ –
Energy lowered

No H3 molecule.

No room for a “third” electron in
the $n=1$ shell

Spin “up” & “down” share $n=1$ level:
Form H$_2$ with less energy than 2H
Covalent bonding

Hydrogen: $^1\text{H}$
- $2s$, $2p$
- $1s$

Helium: $^2\text{He}$
- $2s$
- $1s$

Lithium: $^3\text{Li}$
- $2p$
- $2s$
- Top spin could be “up” or down

Note: Helium is stable -- it is impossible to add an electron into the $2s$ state (Pauli).

Next stable element fills $2s + 2p$
- (need 10 electrons => 10 protons i.e. Neon)

Neon: $^{10}\text{Ne}$
- $2p$
- $2s$
- $1s$

○ represent “empty state”
Ionic bonding

A second way of bonding:

\[ ^{11}_{\text{Na}} \]

\[ 1s \]
\[ 2s \]
\[ 3s \]
\[ 3p \]

\[ ^{17}_{\text{Cl}} \]

(Recall 3d is with 4s and 4p)

one “extra” electron

one “missing” electron
**Ionic bonding**

A second way of bonding: electrons transferred to complete the shells

<table>
<thead>
<tr>
<th>Na&lt;sup&gt;+&lt;/sup&gt;</th>
<th>Cl&lt;sup&gt;-&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>11Na</td>
<td>17Cl</td>
</tr>
<tr>
<td>3p</td>
<td>2p</td>
</tr>
<tr>
<td>2s</td>
<td>1s</td>
</tr>
<tr>
<td>(Now attracted by electrostatic attraction)</td>
<td></td>
</tr>
</tbody>
</table>
We have seen that the different alignment of spins give rise to different atom-atom potentials:

**General pattern:**
1) More atoms => more levels closely spaced.
2) Levels cluster into “bands” with large gaps between them.
Electron bands

This box \((cell)\) repeated \(\sim 10^{23}\) times!

Leads to many levels close together in a “band”

\[
\begin{align*}
2s & \quad \text{2s} \\
\text{“bands”} & \quad \text{“(band) gap”} \\
1s & \quad \text{1s}
\end{align*}
\]

Many atoms
One atom

We get the \textit{band names} from the atomic orbital they split from

\textbf{Filling orbitals before large gap \(\Rightarrow\) inert element (atom-atom bonding)}

is analogous to:

\textbf{Filling bands before large gap \(\Rightarrow\) non-conductive element}

Why? To conduct electrons have to move freely -- means being able to move around in “unoccupied levels”.
Metals vs. Insulators

**Metals**

- Electrons *partially* fill a band
- Lots of states that don’t require much energy to get into
- => Does not take much energy to move an electron
- Metals conduct electricity

![Diagram of Metals]

**Insulators**

- Electrons *completely* fill a band
- Hard for electrons to move, have to apply a lot of energy to get into unoccupied state.
- Insulators do not conduct electricity

![Diagram of Insulators]
Metals vs. Insulators vs. Semiconductors

**Metals**

```
2s
("band) gap"
1s
```

**Insulators**

```
2s
("band) gap"
1s
```

**Semiconductors**

```
1s
```

With “doping” semiconductors can be turned into conductors.
Conducting properties can be tailored by doping

Take Si: Si has 4 electrons on the outermost “shell”=quantum level/orbit
Electrons do not go far from atom

Put P in it: 5=4+1 electrons
P donates extra electron to crystal, can move around freely

Put in Boron: 3=4-1 electrons. Si electrons can fill the “hole” on the B

We can say that in fact, that the hole moves around
Hole is absence of electron: “positively charged”
Diodes

Current through interface

No current through interface

Applying + voltage to n portion switches off current:
Diode rectifies current from AC to DC
(most electrical and computer applications need this)
The Transistor ("transfer resistor") is:

1) **A switch**
   - Digital technology: everything is represented in 1’s and 0’s: open or closed tr.

2) **An amplifier**
   - A small current/voltage controls a much larger current. Signal through many elements **decays**: transistor **re-amplifies** signal: lot of elements can be put together into vast circuits.

1947  Bardeen, Shockley, and Brattain:
   - point contact, bigger than quarter. Basic research lead to discovery

1951  Shockley: p-n-p transistor (different layout)
   - Came to Stanford from East Coast, founded Shockley’s Associates

1958  Fairchild: Integrated Circuit (Shockley, Moore, Hoerni, Noyce)

1968  Intel: Microprocessor  (Moore, Noyce, Shockley, Grove, and Vadasz)
Transistors

Bardeen, Shockley, Brattain (1947)
Integrated Circuit

Integrating more than one element
(Texas Inst.) Kilby 1958: resistor + transistor + wires in air
(Fairchild) Noyce 1959-62: 2 transistors + connections integrated into substrate, no wires in air

Huge litigation, Fairchild won:
Fairchild connection was really “integrated”
Microprocessor

Chips were initially for specific purpose
Ted Hoff (Intel): let’s make it programmable
so it can perform different functions.

First IC (1971): Intel 4004 - 2300 transistors
Today: Intel Core Duo - 800 million transistors
Summary

• **Periodic table:** chemistry controlled by the # electrons in the outer shell = # of protons in nucleus

• **Chemistry =**
  - *Schroedinger* Energy levels (depend on both n and l)
  - *Pauli* exclusion principle

• **Chemical bonding:** All molecules want to lower their energy
  - covalent (shared electrons)
  - ionic (exchanged electrons, electrostatic attraction)

• **Band structure:** Energy level structure of multiple atoms

• **Materials classified according to conduction**
  - metals
  - insulators
  - semiconductors

• **Hole:** An empty state moving around.

• **Diode:** rectifies current

• **Transistor:** switch & amplifier

• **Microelectronics**