Periodic Chart reflects this structure:
show chart from Krane

Properties of chemical elements can be understood in terms of the Atomic level structure we are discussing.

- Filled subshells, very stable configurations
  - Normally do not contribute to "chemistry"
- Atoms having 1e⁻ over a filled shell will readily give that e⁻ up in a chemical reaction (lower overall energy).
- Atoms lacking 1e⁻ from a filled shell will react to gain that e⁻ to form a filled shell (more stable).

See Krane Fig 8.4 p 210

Measure of ease with which
1e⁻ is given up.

low = easy
high = hard.

KRANE 8.3 p 209

As Z increases within a shell, atomic radius decreases.

As new shell is added, atomic radius increases.

Bohr Atom $R = \frac{n^2}{Z}$
- H, Na are very reactive.
- Noble gases He, Ne, Ar... have filled levels and are very inert chemically.

**Chemical bonds**

**Ionic bond** - one atom takes an electron from another = both have filled shells (more stable) and are charged (attract each other)

\[
\begin{align*}
Z=11 & \quad \text{Na} \quad [\text{Ne}]^{3s^1} \\
Z=17 & \quad \text{Cl} \quad [\text{Ne}]^{3s^23p^5}
\end{align*}
\]

\[\text{Na}^+ \quad [\text{Ne}] \quad \text{ions} \quad \text{Attract each other (electrostatic)} \quad \text{NaCl} \quad \text{Table salt}
\]

**Covalent bond**

\[\text{H}_2\]

Each H shares 2 electrons \(\rightarrow\) Molecular orbital

\[\begin{align*}
&\text{H} \quad \text{H} \\
&\text{High electron density in the middle}
\end{align*}\]

\[\text{H} - \text{C} - \text{H} \quad \text{Methane} \quad (\text{C needs 4 e\textsuperscript{-} to get to [Ne]})
\]

\[\text{H}\quad \text{H} \quad (\text{H needs 2 e\textsuperscript{-} to get to [Ne]})
\]
Spectroscopy

Discrete energy levels

Key to understanding Atomic Structure

Transitions occur between allowed STATES

Permits a detailed study of atomic model, environment of atom, sample composition (NMR) (EPR) (emission, absorption spectra)

Many applications: X-rays, NMR, lasers ...

X-rays

1895 discovery Roentgen

\[ E \]

\[ E \]

Cathode tube

Cathode rays

\( e^- \) incident on a high Z material \( n=\infty \)

\( X\text{-rays} \)

\[ 100 \sim 100,000 \text{ eV} = h \nu \]

Overlaps ultraviolet on the soft end and gamma rays on the hard end

\[ n=3 \]

M shell

\[ n=2 \]

L shell

\[ n=1 \]

K shell
ion Principle - Chemistry, Biochemistry explained by quantum mechanics.
- Forces at work basically understood

$\Rightarrow$ Chemists, Biologists not out of business
  - Cannot solve QM of complex systems like medium sized molecules or dogs.
  - New and unexpected phenomena come about with added complexity $\Rightarrow$ life

Key to understanding Atomic Structure experimentally is Spectroscopy.

Many different kinds

optical transitions occur in relatively loosely held outer shells

E.g., $\underline{5s} \rightarrow 4d$ Re $\rightarrow 427 \text{ nm}$

must obey selection rules

conserves angular momentum and spin.

X-rays occur when tightly bound inner electron in high Z electron is ejected and one of the outer electrons makes a transition down to the lower shell

$\underline{5s} \rightarrow 4d \rightarrow 4p \rightarrow 4s \rightarrow \underline{3d}$

$n=1$ K Shell
Calculate the energy necessary to "ionize" heavy elements with $Z = 40$ by removing $e^-$ from $n=1$ shell

$$E_n \sim -\frac{Z^2}{n^2} E_0 \sim -40^2 (13.6 \text{ eV}) \approx 22000 \text{ eV}$$

This is the order of magnitude for $E_{\text{hv}}$ emitted as electrons from outer shells cascade down to fill the hole.

X-rays also from high intensity light sources

\[ e^- \rightarrow \quad \text{NSNSN} \quad \text{NSNS} \quad \text{undulating} \quad \text{Magnet} \]

from above

\[ \text{frequency determined by } P_0 \text{ and spacing of } \text{Magnets} \]

Very important source of high intensity, high frequency electron-beam x-ray beams for research.

We will discuss absorption when we do Nuclear Physics.
Electron Spin Resonance (ESR)
Nuclear Magnetic Resonance (NMR)

Recall

Particles can be thought of as "spinning" charge distributions or quantize "allowed" values of Angular frequency

$e^-$ point-like as far as we know

$\Rightarrow$ Nuclei have structure

This is intrinsic Spin $\Rightarrow$ leads to a small magnetic moment acts like a small Dipole

\[ S_z \]

Intrinsic Angular Momentum $I$

Total Spin $\frac{1}{2}$ for $e^-$

Integers $I$ for nuclei

$\frac{1}{2}, 1, \ldots$ etc.

Spin $z$ component

$M = I, I-1, \ldots -I$

$e^- \pm \frac{1}{2} = MS$

Nuclei also $\pm$ value

Determining Spin Structure is important in Nuclear Structure Expts

Spin can also be used as a diagnostic or tool for probing particle environment
Dipole in Magnetic Field

Potential Energy in system
Depends on the orientation of Dipole in B field
let z direction be along B

\[ E_{\text{mag}} = -g \mu B m_z \]

\[ \text{E magnetic}

\text{(NOT writing)}\]
\[ \text{Magnetic}
\text{Moment of particle}\]

For \( B=0 \)

atoms/nuclei up all \( M \) at in a given energy level are degenerate in energy

Atom \( N=3 \) \( l=1 \) \( M_l = \frac{1}{2}, \frac{3}{2} \) all have same energy

\[ m_s = \pm \frac{1}{2} \]

Turn on B

Split due to B

Zeeman splitting

If an unpaired electron present

get additional split

due to \( e^- \) spin-B interaction
Spectroscopy in Magnetic fields / Electric fields: important tools!

Zeeman Splitting

Recall $E = \hbar \omega$

Little magnetic dipole created by $e^-$ orbiting around nucleus

$$M_e = \frac{M_b}{\hbar} \vec{L} = \left( \frac{e}{2M} \right) \vec{L}$$

Suppose we have an atom with $e^-$ in 2p state ($\text{ignore } e^- \text{ spin}$)

Energy of interaction of $M$ with $B = \nu = -M \cdot \vec{B}$

Let direction of $B$ determine $Z$ axis

Then

$$\nu = \left( \frac{e}{2M} \right) \vec{L} \cdot \vec{B} = \frac{e}{2M} L_z B = \frac{e \hbar}{2M} M_e B = M_e \frac{e \hbar}{2M}$$

2p state $M_e = 1, 0, -1$

$m_L$ values degenerate

\[ \text{Field off} \]

\[ \text{Field on} \]

\[ \Delta T = \frac{h \omega}{M_e B} \]

\[ h \omega = h \nu = h \frac{e \hbar}{2M} \]
Transitions between energy levels could occur at a different frequency.

Usefulness in chemistry, biology:

Atoms with dipole fields

Nuclei:

Typical NMR

Put sample in B field

Estate of depends on orientation of spin ½ protons with respect to B

Apply hν to cause transitions between two relative spin levels

Exact hν depends on B0f and depends on "Nuclear Environment"