Forces between atoms and molecules
Elements whose outer shells are not filled are chemically reactive.
Pauli exclusion principle and the Periodic Table of elements

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Covalent bonding

Hydrogen atoms (H)

Electrons attracted by each others’ protons

Covalently bonded hydrogen molecule (H₂)

O₂

F₂
Properties of covalent compounds

Strong covalent bonding forces within molecules

Gaseous phase

Liquid phase

Weak nonbonding forces between molecules

A Quartz

Silicon

Oxygen

B Diamond

Carbon
Ionic bonding

Metals like Na tend to lose electrons. Non-metals like Cl tend to gain electrons.

Sodium
11 electrons
Covalent radius 0.154 nm

Losing 1 electron drops Na back to a stable 2s2p octet like the noble gas neon.

Chlorine
17 electrons
Covalent radius 0.099 nm

Gaining 1 electron fills the stable 3s3p octet like the noble gas argon.
NaCl – an ionic crystal where ions are bound by ionic bonds
Modern periodic table

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Electron Cloud Distribution

Uniform distribution of electron cloud about the nucleus.

Non-uniform distribution of electron cloud - separation of + and - charge within atom.
Permanent dipole moment in **polar molecules**

- **HF (Hydrofluoric Acid)**
- **H₂O (Water)**
- **CO₂ (Carbon Dioxide)**

Dipole – dipole interaction
Hydrogen bonding

- Hydrogen bond between water molecules
- Hydrogen bonds in ice
- Ice → Melting → Water
An electron orbiting a proton in Hydrogen atom – flickering dipole
Oscillating dipoles radiate – electric field

The real-time evolution of the electric field of an oscillating electric dipole is shown. The dipole is located at (60,60) in the graph, oscillating at 1 rad/s (~.16Hz) in the vertical direction.

Most of the interactions between atoms can be expressed in terms of inverse power laws of the distance, \( r \). In most cases these analytical expressions are given in terms of \textbf{potential energy} of the interaction, \( U(r) \).

Note that force is the negative gradient of the potential energy:

\[
F(r) = -\frac{dU(r)}{dr}.
\]

- Coulomb potential: \( \sim \frac{1}{r} \)
- Charge – dipole interaction potential: \( \sim \frac{1}{r^3} \)
- Dispersion interaction potential: \( \sim \frac{1}{r^6} \)
- Repulsion between electronic clouds at short distance: \( \sim \frac{1}{r^{12}} \).
Dipole-Dipole

\[ E = -\frac{\mu^2}{4\pi \varepsilon_0 r^3}, \]

where \( \mu = q \cdot l \), the dipole moment.

Dipole-Induced Dipole

\[ E = -\frac{2\alpha \mu^2}{(4\pi \varepsilon_0)^2 r^6} \]

where \( \alpha \) is the polarizability.

London Dispersion Forces

\[ E = -\frac{3\alpha^2 \hbar \omega_0}{4(4\pi \varepsilon_0)^2 r^6}. \]

Hydrogen Bond

Special Case of Dipole-Dipole

O—H or N—H near O, F, N, or Cl.
Pauli exclusion principle

No two electrons can have the same values of all four quantum numbers.

Two electrons, and more generally two fermions, cannot have the same quantum state (position, momentum, mass, spin).

Pauli repulsion
Different terms are most important for describing the interaction between different atoms and molecules. In particular, the interaction between noble gas atoms is well described by the potential energy function, which has Lennard-Jones name:

$$U(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right]$$

Here $\epsilon$ and $\sigma$ are parameters determined from experimental data.

For Argon, $\epsilon = 0.0104$ eV and $\sigma = 0.340$ nm
Fig. 2.6. (a) A thought experiment in which the position of the left-hand atom is fixed. The right-hand atom may be set various distances $r$ (measured between centres) from the left-hand atom and the force of attraction (or repulsion) 'read' on a Newton balance. (b) The general form of the interatomic force between the two atoms of (a). Note that negative forces are plotted along the upward ordinate and positive forces along the downward ordinate. (c) The corresponding variation in potential energy.
Potential energy curve for $\text{H}_2$ molecule
Ne\textsubscript{2} molecule