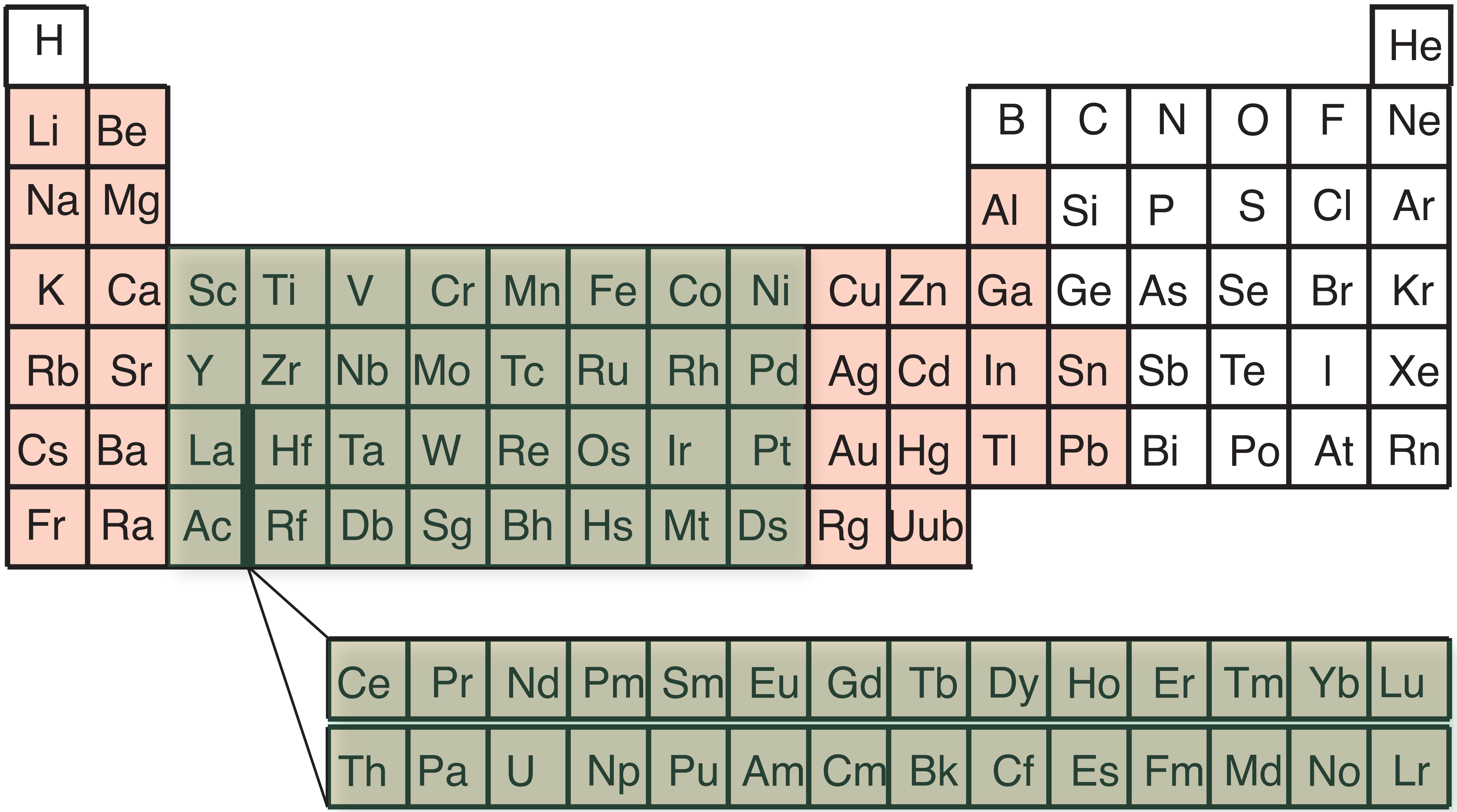
Condensed Matter Physics

Metallic bonding

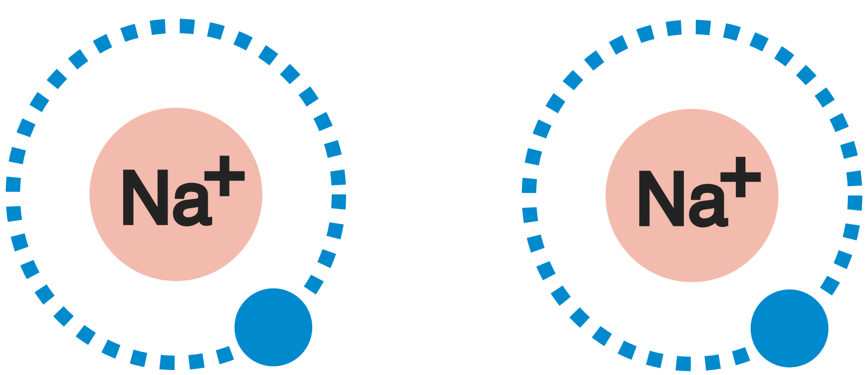
metals / non-metals

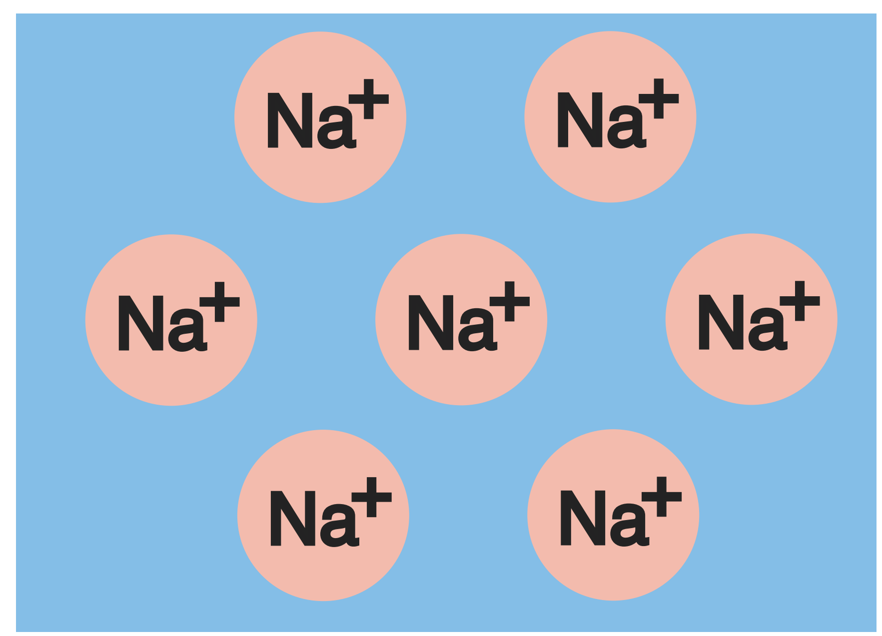


- the boundaries can be disputed
- simple metals, transition metals, noble metals

Metallic bonding (simple metals)

- outer electrons are delocalized and act as “glue” between positively charged ion cores
- generally found for elements with one, two or three valence electrons.
- cohesive energies in the eV range





Metallic bonding (simple metals): more characteristics

- smaller cohesive energies than in ionic crystals
- larger ionic radii, e.g. for Na: 3.82 Å (metal) and 1.94 Å (NaCl)
- bonding has no directional preference
- closed-packed atomic configurations are preferred: best possible overlap between the orbitals, no “holes” in the potential

Metallic bonding: why is this so favorable?

$$-\frac{\hbar^2\nabla^2}{2m}\Psi(r) + U(r)\Psi(r) = E\Psi(r)$$

kinetic energy (or Hamiltonian for a free particle)
$\propto$ (negative) average curvature of wave function
"flatter" wave function -> lower energy

$$\Delta x \Delta p \geq \hbar/2$$

less localization -> smaller p variation

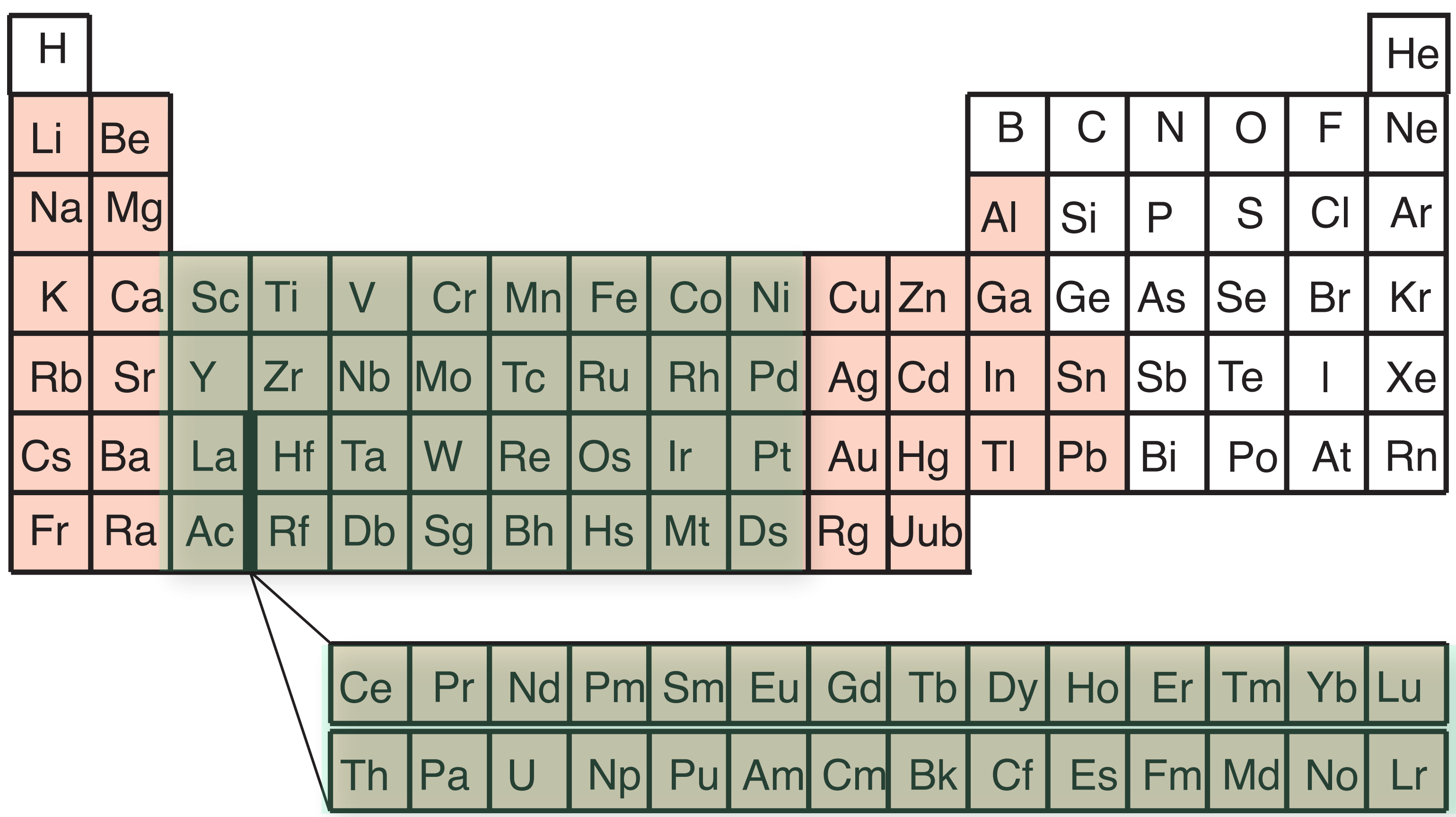
Metallic bonding: why is this so favorable?

$$-\frac{\hbar^2\nabla^2}{2m}\Psi(r) + U(r)\Psi(r) = E\Psi(r)$$

image source: wikipedia

Transition metals

- 4s and 3d have very similar energies
- 4s electrons form delocalized metallic bonds
- 3d electrons form more local (covalent-like) bonds
- higher cohesive energies



Bonds between molecules

- molecular solids are very common (but not at RT)
- ice
- plastic
- DNA
- what makes molecules bond to each other?

Bonds between molecules: hydrogen bonds

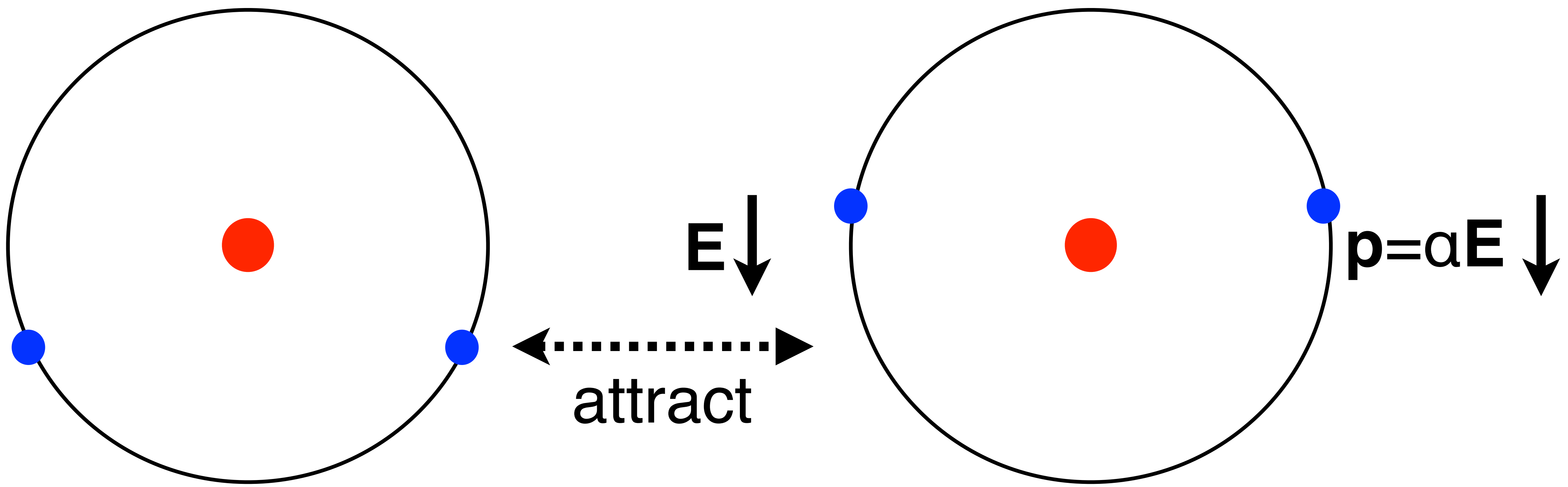
permanent dipole

Bonds between molecules: hydrogen bonds

- H is positively charged but also very small: another “real” bond cannot be established without overlap of electron clouds (in this sense it is too big in this drawing).
- H bonding is important in ice, DNA... but not very strong

Bonds between molecules: van der Waals force

$$U = -\mathbf{E}\cdot\mathbf{p} = -\mathbf{E}\cdot\alpha\mathbf{E} \propto -\frac{1}{r^3}\alpha\frac{1}{r^3}$$



- dipole moment caused by fluctuations
- this is always present as an attractive force (even between He atoms as in this case)
- it is very weak and depends on the distance as r^{-6}

Bond type and physical properties

- How does the bond type affect the properties of a solid such as:
- mechanical strength / melting point
- electrical conductivity
- thermal conductivity
- optical properties

Bond type and physical properties

Summary

- We have looked at different types of bonding: ionic, metallic, covalent, H-bonds, van der Waals bonds.
- In reality, intermediate bonding scenarios are often found.
- We have some ideas about the relation between between the bonding type and the physical properties (at least for the melting point).