<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
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<tr>
<td>Ionization energy</td>
<td>Na → Na⁺ : 5.14 eV</td>
<td>Table 5</td>
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<tr>
<td>Electron affinity</td>
<td>Cl → Cl⁻ : 3.61 eV</td>
<td>Table 6</td>
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<tr>
<td>Madelung Constant NaCl</td>
<td>α = 1.797565</td>
<td>p. 65</td>
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<tr>
<td>Rₖ nearest neighbor distance</td>
<td>= 2.820 Å</td>
<td>Table 7</td>
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<tr>
<td>S repulsive parameter</td>
<td>= 0.321 Å</td>
<td>Table 7</td>
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</table>

Ionic energy:

\[
U = \sum \left[ -\frac{q_i q_j}{R} + 2 \frac{Z_i Z_j e^2}{R^s} \right]
\]

Coulomb energy:

\[
\frac{-k_e q^2}{R_0} = -5.1063 \text{ eV}
\]

\[
k_e = 8.987 \times 10^9 \ldots \quad q = e = 1.60219 \times 10^{-19} \text{ C}
\]
Madelung energy \[ = -\frac{keq^2}{R_0^2} = -8.9236 \text{ eV} \]

Lattice energy \[ = -\frac{keq^2}{R_0} \left[ 1 - \frac{q}{R_0} \right] \]  

\[ \text{Eq 3.2a} \]

\[ V \text{ at minimum} \]

\[ \text{This is the difference between} \]

\[ \text{Na}^+ \leftrightarrow \text{Cl}^- \text{ and } \text{NaCl} \]

Cohesive energy \[ = |\text{lattice energy}| - \text{ionsization energy} + \text{electron affinity} \]

\[ = +7.9078 \text{ eV} - 5.14 \text{ eV} + 3.61 \text{ eV} \]

\[ = 6.378 \text{ eV} \]
Covalent Crystals

Bond is formed from 2 electrons, one from each atom.

Electron spins are antiparallel ↑↓ (Pauli exclusion)

Covalent bonds are very strong like ionic bonds, not like the weak van der Waals bonds.

Real materials - bond is some fraction ionic, some fraction covalent.

Covalent bonds are highly directional → low packing fraction 34% vs. 74% for fcc
Exchange interaction
Phonons

Longitudinal wave

Displacements from equilibrium

Transverse wave

Assumptions:
- Nearest neighbor interaction only.
- Force on a given atom is proportional to the displacement. Hooke's law.
Generic Potential

\[ U(r) = U_0 + \frac{dU}{dr} (r - r_0) + \frac{1}{2} \left( \frac{d^2U}{dr^2} \right) (r - r_0)^2 \]

Taylor expand around minimum

Choose \( r = r_0 \)

at minimum \( (r - r_0)^2 \)

\[ = C U^2 + \ldots \]

\[ \uparrow \text{spring constant} \]

Force on an atom in the s-plane

\[ F_s = C (u_{s+1} - u_s) + C (u_{s-1} - u_s) \]

\[ M \frac{d^2u_s}{dt^2} = C \left[ u_{s+1} - 2u_s + u_{s-1} \right] \]
Difference (not differential) equation.

Expect sinusoidal waves 
time dependence \( e^{-i\omega t} \)

\[ U_s \propto e^{-i\omega t} \quad \frac{d^2 u_s}{dt^2} = -\omega^2 e^{-i\omega t} \]

Time part

\[ M \frac{d^2 u_s}{dt^2} = C \left[ U_{s-1} - 2U_s + U_{s+1} \right] \]

\[ -M \omega^2 u_s = C \left[ U_{s-1} - 2U_s + U_{s+1} \right] \]

Space part

\[ u_s = A e^{i k x_s} = A e^{i k a s} \]

\[ U_{s+1} = A e^{i k a(s+1)} = A e^{i k a s} e^{i k a} \]

\[ U_{s-1} = A e^{i k a s} e^{-i k a} \]