Electronic properties of selected materials (G and P Ch. VI)

- Noble gas solids:

* Examples: Ne, Ar, Kr, Xe
* Crystal structure: FCC
* Bonding: Individual atoms have filled shells, bond via van der Waals interactions
* Electronic structure: occupied p, large gap (~10-20 eV) to unoccupied s
* Semi-empirical description: Lennard-Jones potential

Pairwise interaction, interatomic distance R

$$U(R) = \varepsilon\left[\left(\frac{\sigma}{R}\right)^{12} - 2\left(\frac{\sigma}{R}\right)^{6}\right]$$

$\left(\frac{\sigma}{R}\right)^{12}$: hard sphere repulsion

$\left(\frac{\sigma}{R}\right)^{6}$: van der Waals attraction

- Ionic crystals:

* Examples: LiH, NaCl, ZnO, GaN
* Crystal structure: various including rock salt, cesium chloride, zincblende, wurtzite (see G and P Ch. II)
* Bonding: Atoms fill shells by charge transfer, interact via Coulomb interaction
* Electronic structure: various, but often wide band-gap insulators
* Semi-empirical description: Sum of alternating charges

nearest neighbor distance

$$U(R) = N\left(\frac{1}{R^{n}} - \alpha_m \frac{e^2}{R}\right)$$

N: number of positive/negative ions

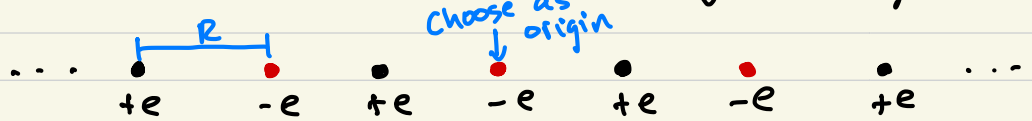
$\frac{1}{R^n}$: repulsion

α_m: Madelung constant

$\frac{e^2}{R}$: point charge attraction

- Madelung constant describes sum over point charge interactions

- Consider 1D chain of alternating charges $\pm e$ separated by R:



$$V = -\frac{e^2}{R} 2\left[1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \cdots\right] = -\frac{e^2}{R} 2\ln 2 \equiv -\alpha_m \frac{e^2}{R}$$

↑ converges slowly! challenge in 3D

- <u>Covalent crystals</u>:

  * Examples: C, Si, Ge, Sn

  * Crystal structure: various, including diamond

  * Bonding: Atoms fill shells by sharing electrons

  * Electronic structure: various, insulating, metallic, semiconducting

  * Semi-empirical description: See empirical pseudopotentials (HW 6)

- <u>Simple metals</u>:

  * Examples: Fe, Na, Cu, Li, Pd, Au, Ag, ...

  * Crystal structure: FCC, BCC, HCP

  * Bonding: Atoms fill shells by sharing loosly bound electrons

  * Electronic structure: Metallic (ü), bands crossing Fermi level

  * Semi-empirical description: Uniform electron gas (Jellium model)

$$E_{HF} = \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right]$$ (see Q and P Sec. IV.7)