Lecture #1

2-D Lattice and Unit Cell

Chemistry 484

Spring Quarter, 2006

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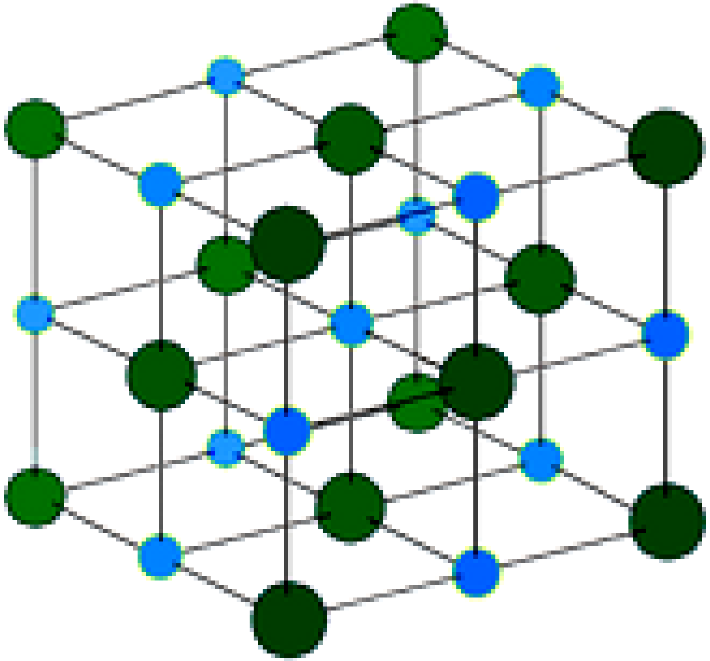
Molecules and Solids (Crystals)

Similarity



Difference

Connection

Periodic Table

1998 Dr. Michael Blaber

← VIII →

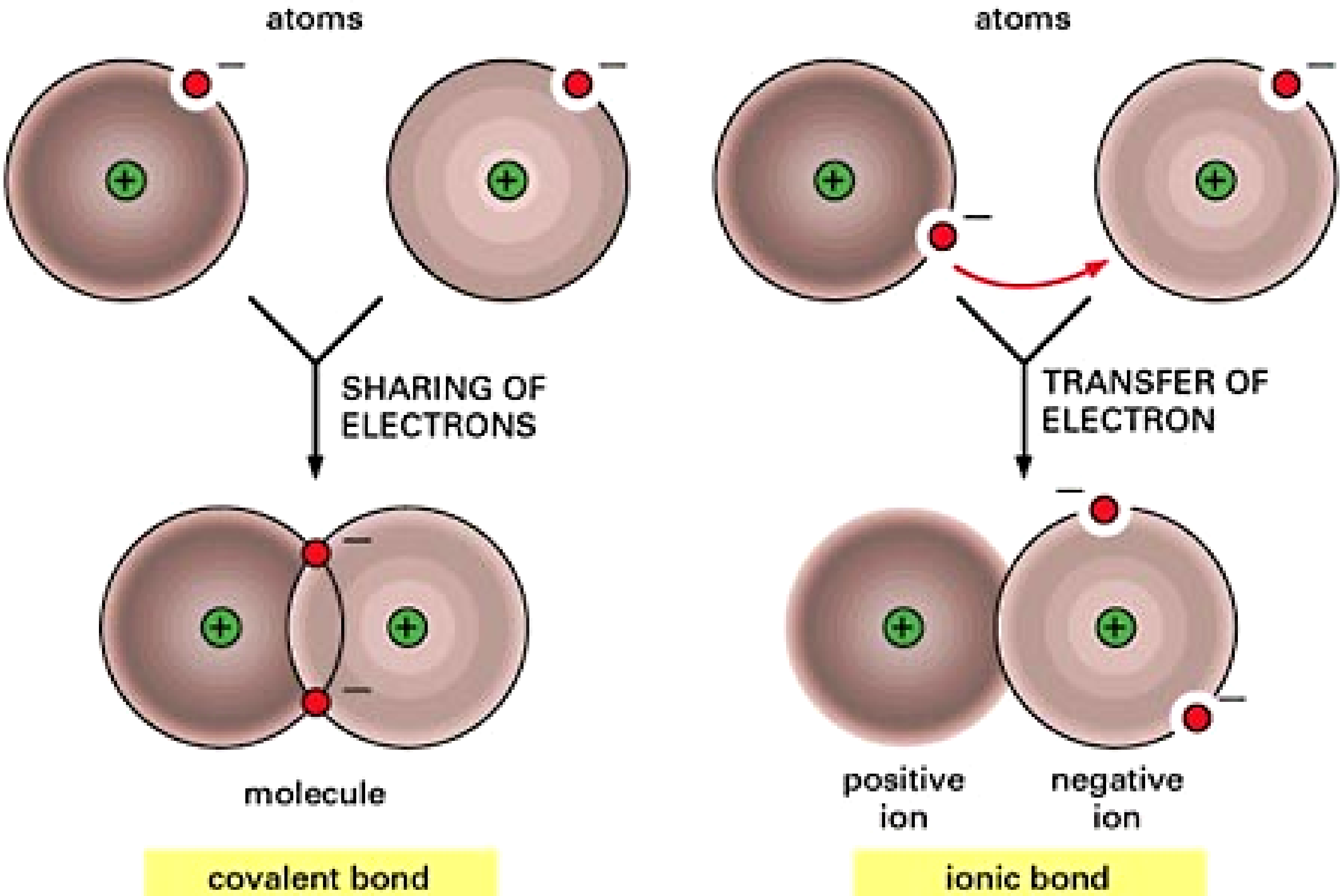
	1/IA	2/IIA	3/IIIB	4/IVB	5/VB	6/VIB	7/VIIB	8	9	10	11/IB	12/IIB	13/IIIA	14/IVA	15/VA	16/VIA	17/VIIA	18/VIIIA
1	1 H 1.008																	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	12 Mg 24.30											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.05	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc 98.91	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 123.9	56 Ba 137.3	La-Lu	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po 210.0	85 At 210.0	86 Rn 222.0
7	87 Fr 223.0	88 Ra 226.0	Ac-Lr	104 Db	105 Jl	106 Rf	107 Bh	108 Hn	109 Mt	110 Uun	111 Uuu							

← *s* → ← *d* → ← *p* →

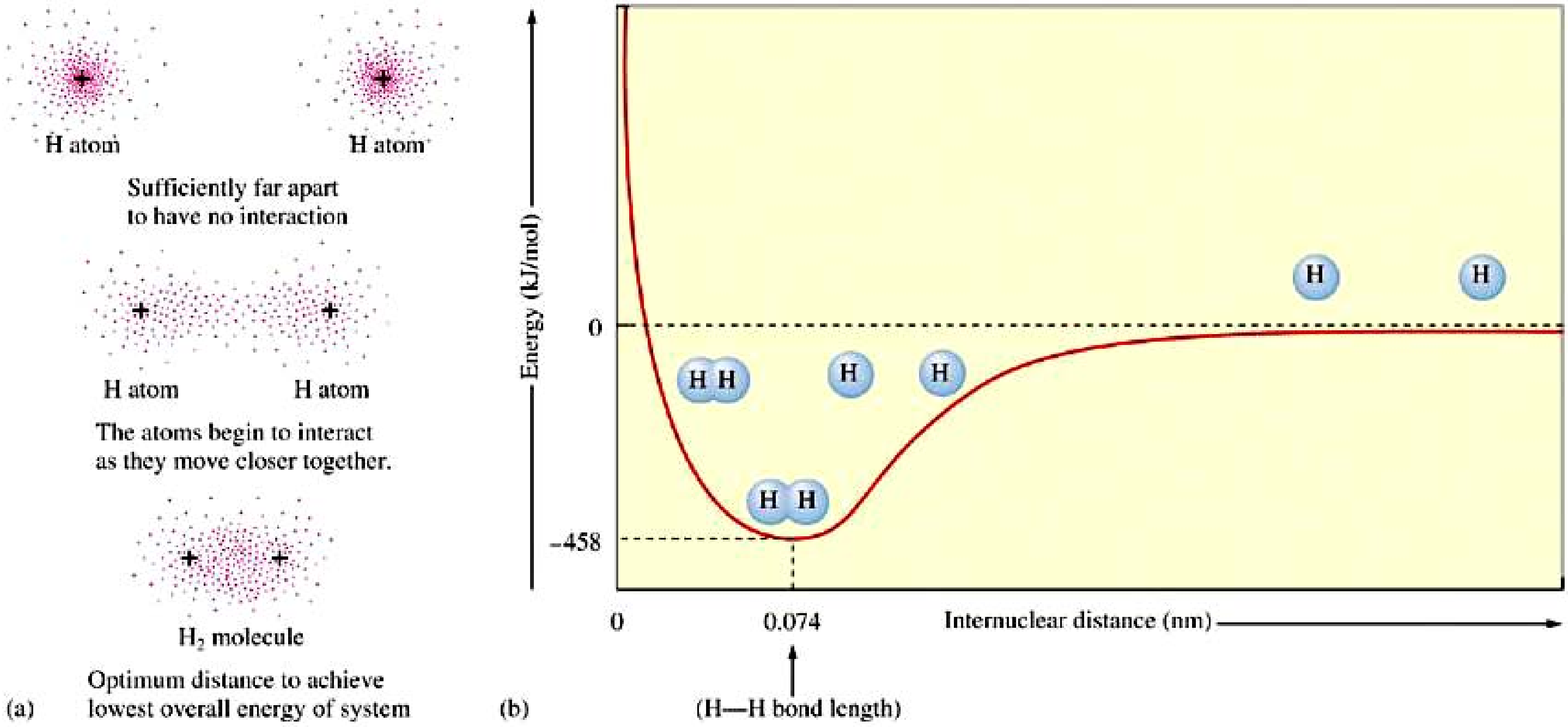
Lanthanides	57 La 138.9	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm 146.9	62 Sm 150.4	63 Eu 152.0	64 Gd 157.2	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
Actinides	89 Ac 227.0	90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np 237.0	94 Pu 239.1	95 Am 241.1	96 Cm 244.1	97 Bk 249.1	98 Cf 252.1	99 Es 252.1	100 Fm 257.1	101 Md 258.1	102 No 259.1	103 Lr 262.1

← *f* →

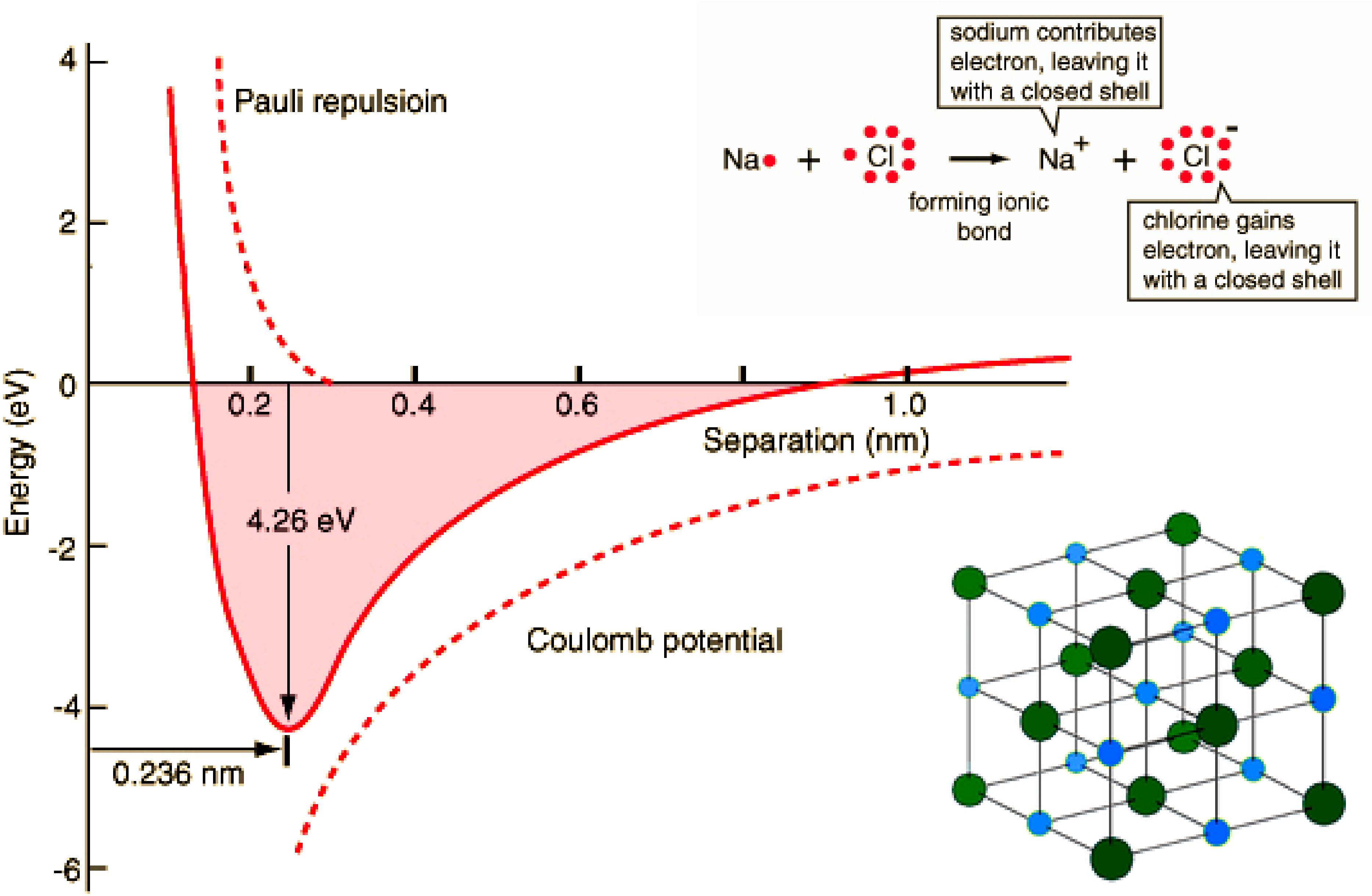
Formation of Chemical Bonds



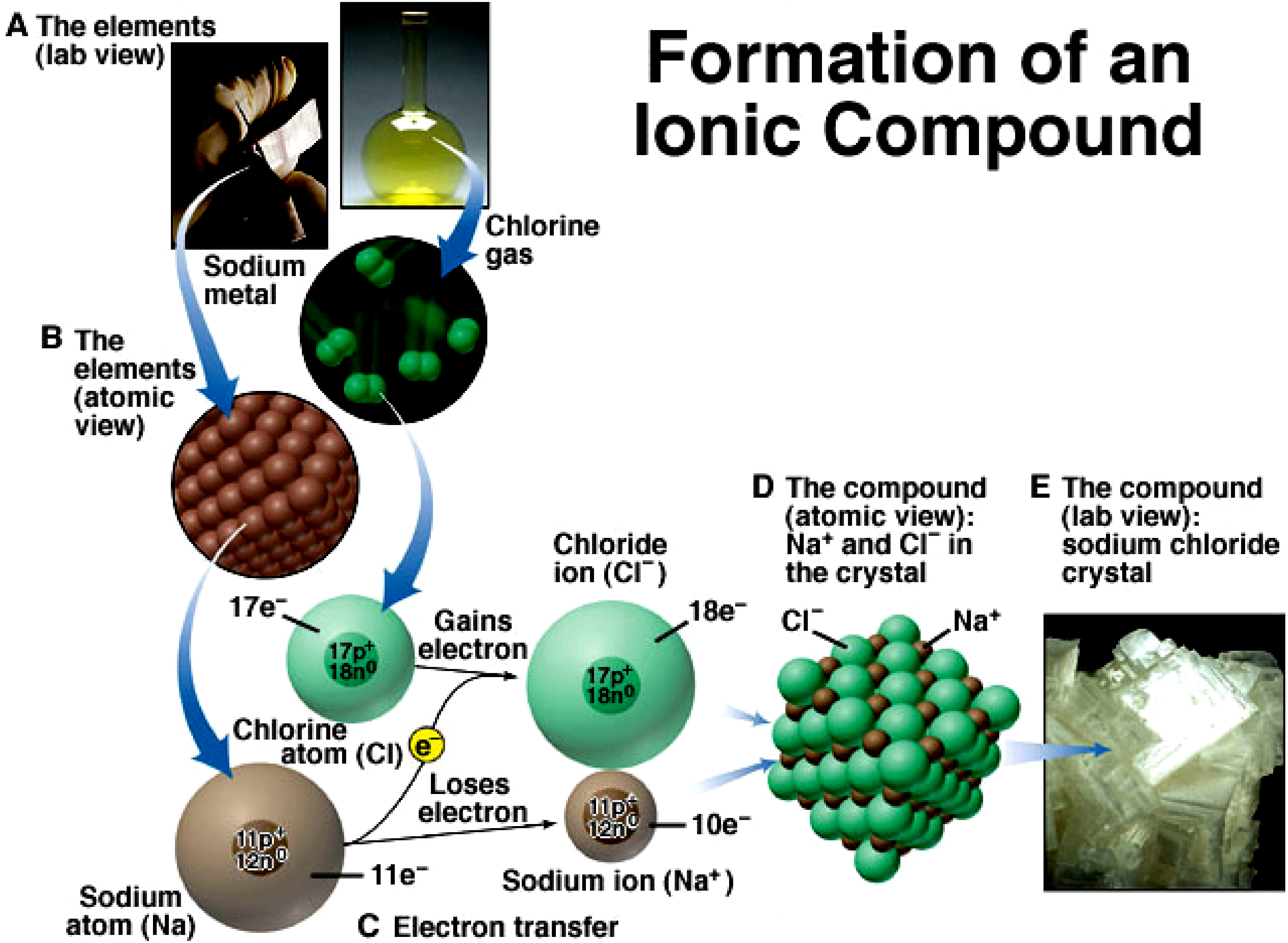
Formation of Covalent Bonding



Formation of Ionic Bonding



Formation of an Ionic Compound



Types of Chemical Bonding

- Covalent Bonding – atoms share electrons to form discrete molecules. Polymers – very large molecules that are made up of many (>5) smaller molecules (monomers) repeatedly linked together.

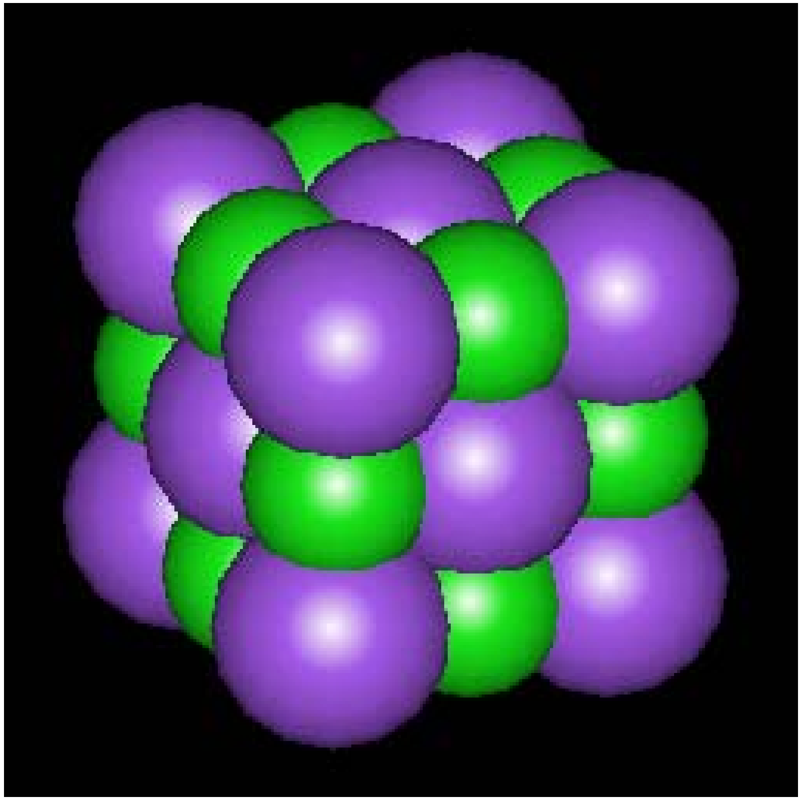
- Ionic Bonding – picks up or loses electrons, ion is charged atom (Na^+) or group of atoms (NO_3^-). The force of attraction between oppositely charged ions (cations/anions) leads to the formation of ionic compounds and solids.

- Metallic Bonding – positive ions in “sea of electrons”.

Discrete Molecule vs. Extended Solid

Element Combination	Likely Structure	Examples
Metal and metal	Extended (metallic)	CuZn (brass), NiTi
Metal and nonmetal	Extended (ionic)	NaCl
Nonmetal and nonmetal	Discrete (molecular) or Extended (covalent network)	$SiCl_4$ (discrete) Si (extended)

Stoichiometry of Extended Solids



rock salt: NaCl

Empirical Formula

How does the crystal structure of rock salt reveal the formula?

Lattice

- A periodic array of “dots” (or lattice points) with infinite repetition. In reality, we have to deal with finite sizes.

- It is a mathematic abstraction used to describe the translational symmetry (or order) of a periodic structure.

- A lattice can be described in terms of unit cell and lattice parameters (constants): (*a, b, c*) and (α, β, γ).

- Crystal Structure = Lattice + Content of the Lattice Point

Unit Cell

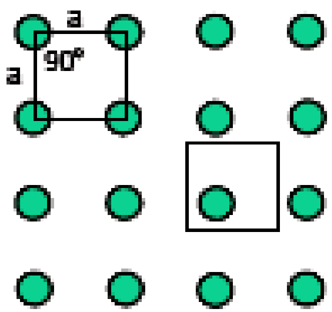
- The simplest portion of a lattice that can be repeated by translation to cover the entire lattice ($\boldsymbol{T} = m\boldsymbol{a} + n\boldsymbol{b}$).

- In general, we choose the unit cell such that it can reflect the symmetry of the original lattice.

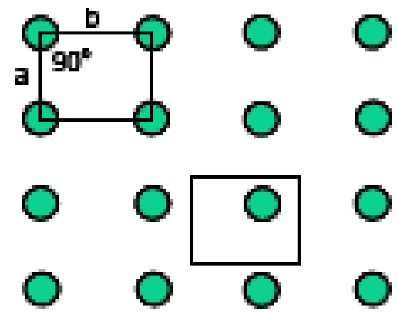
- Primitive cell (P): only contain one lattice point. We must use primitive cells as long as they match the symmetry of the lattice.

- Centered cells: I, C, F

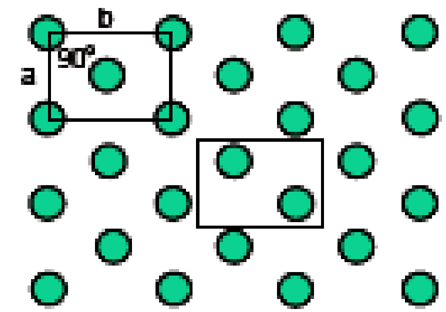
2-D Lattices and Unit Cells



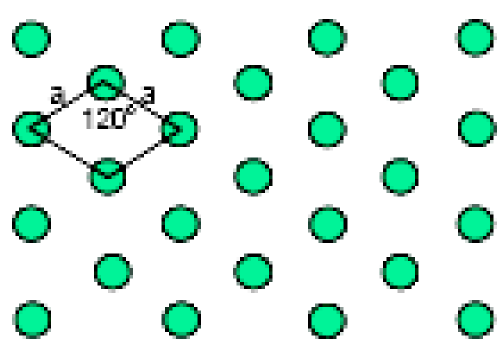
square lattice
square unit cell



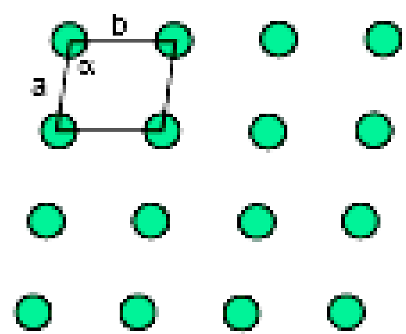
rectangular lattice
rectangular unit cell



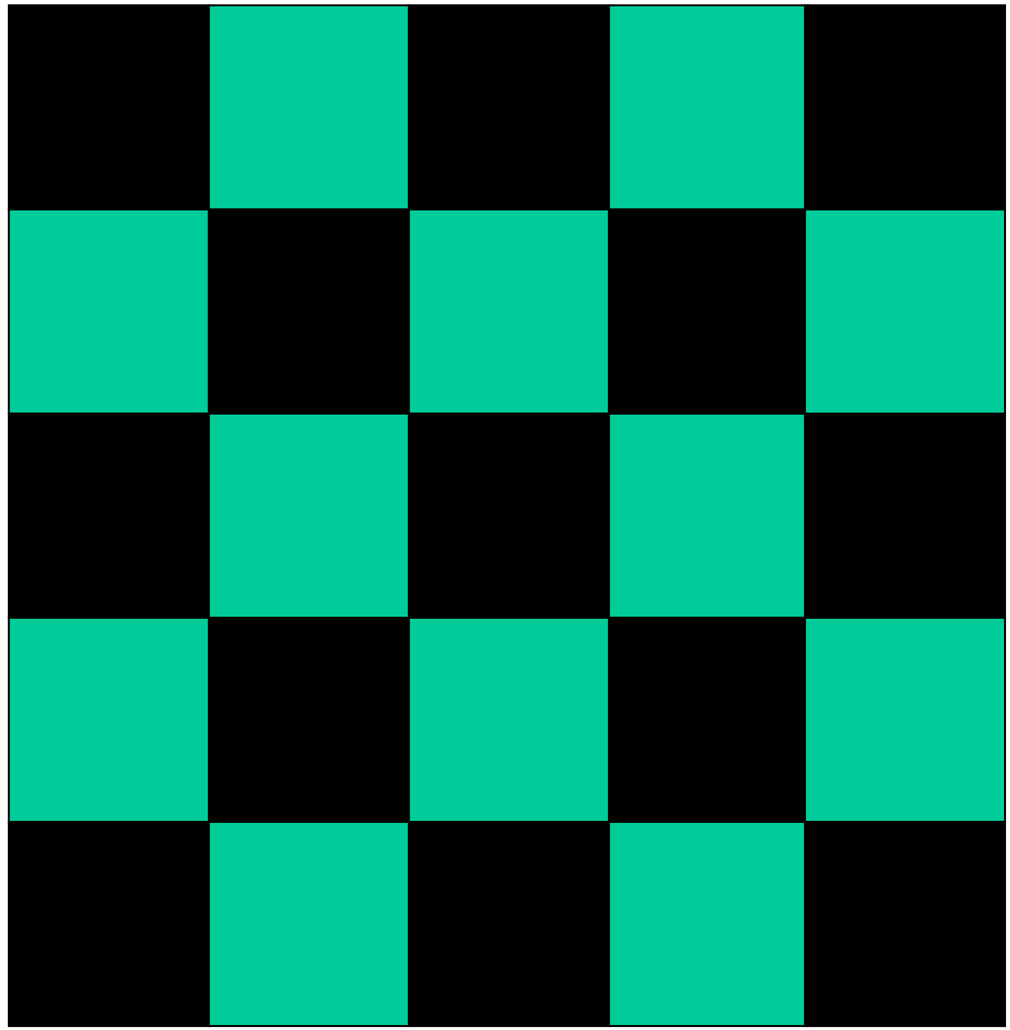
rectangular lattice
centered rectangular unit cell

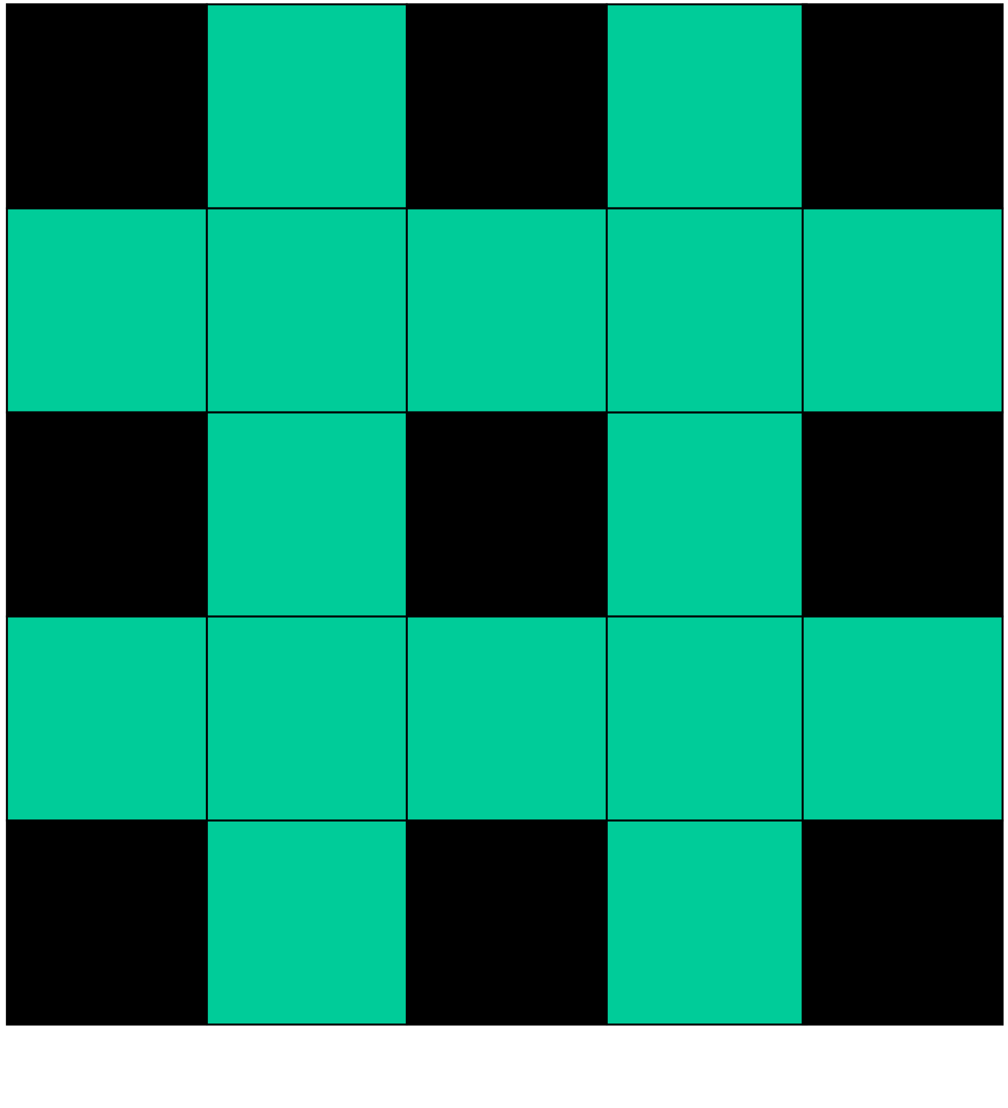


hexagonal lattice, unit cell



parallelogram lattice, unit cell





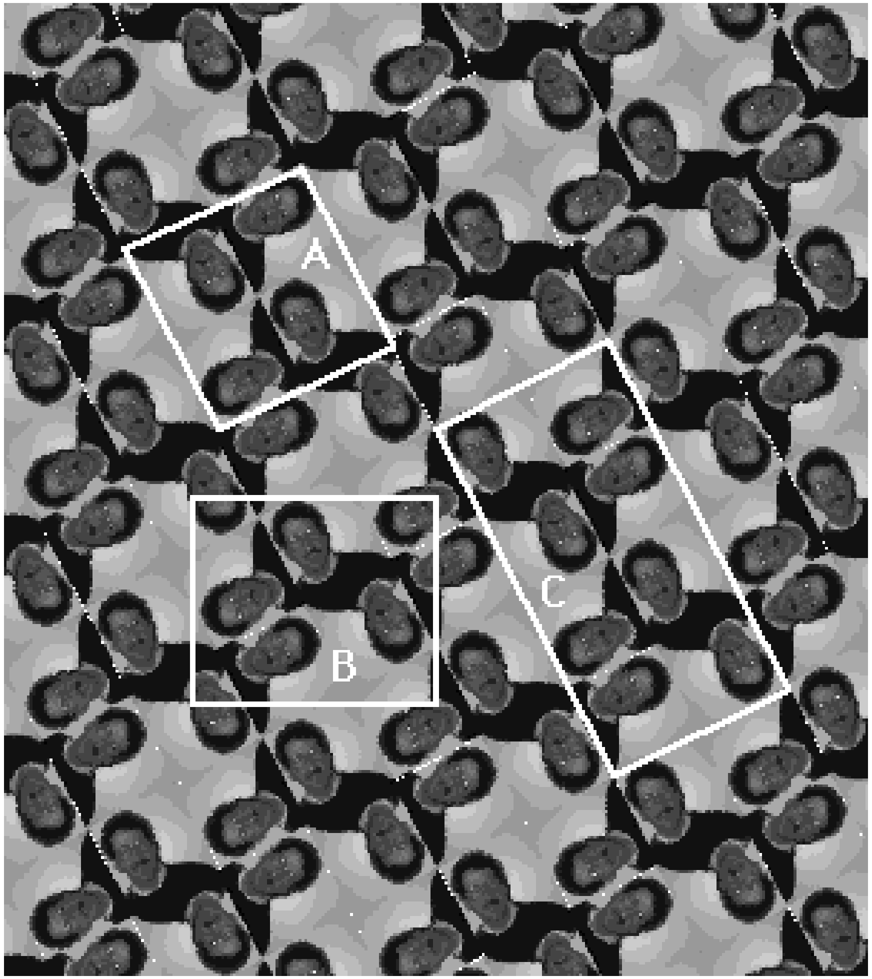
Finding the Unit Cell

Which of the parallelograms in the figure below are unit cells?

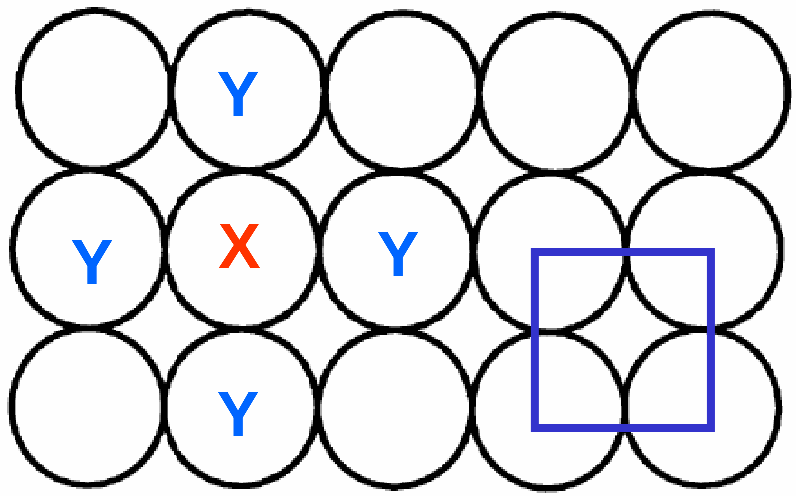
A, B, C

How many total heads are included in the correct unit cell?

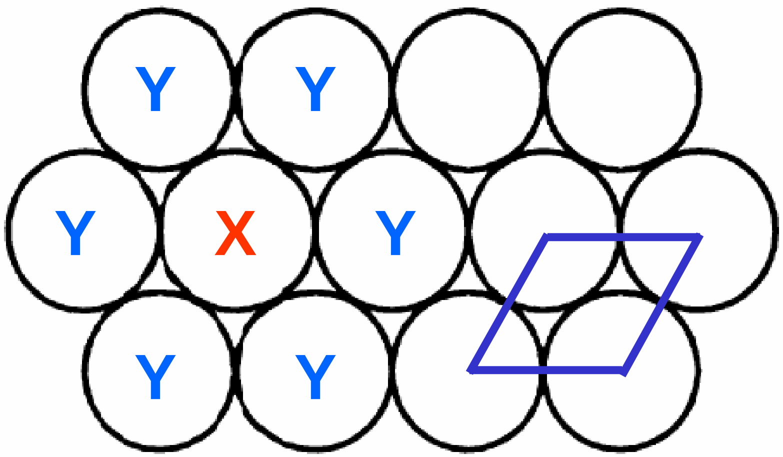
4, 6, 8



Two-Dimensional Packing



square packing (square)
coordination number = 4



close packing (hexagonal)
coordination number = 6

- What is the most efficient way to arrange circles (balls, or atoms) on a plane surface?

Packing Efficiency

$$\%\ \text{packing efficiency} = \frac{\text{Area of circles in unit cell}}{\text{Area of unit cell}} \times 100\%$$

Square Packing: ~79%

Close Packing: ~91%