IKATAN KRISTAL (CRYSTAL BONDING)

Rita Prasetyowati
Fisika FMIPA UNY
2012

- These are weak bonds with a typical strength of 0.2 eV/atom.
- Van Der Waals bonds occur between neutral atoms and molecules.
- Weak forces of attraction result from the natural fluctuations in the electron density of all molecules that cause small temporary dipoles to appear within the molecules.
- It is these temporary dipoles that attract one molecule to another. They are called van der Waals' forces.

Energi interaksi dalam ikatan Van der Waals :

$E(r) = -A/r^6 + B/r^{12}$

Dirumuskan lebih lanjut oleh Lennard-Jones dalam bentuk :

$E(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r^6]$ ➔ *energi potensial Lennard-Jones*

Ikatan Ionik

Ikatan ionik terbentuk karena adanya gaya tarik-menarik elektrostatik (Coulomb) antara ion positif dan ion negatif.

Transfer elektron → terbentuk ion

Contoh kristal ionik :

NaCl, CsCl, KBr, NaI, dst.

IONIC BONDING

- Ionic bonding is the electrostatic force of attraction between positively and negatively charged ions (between non-metals and metals).

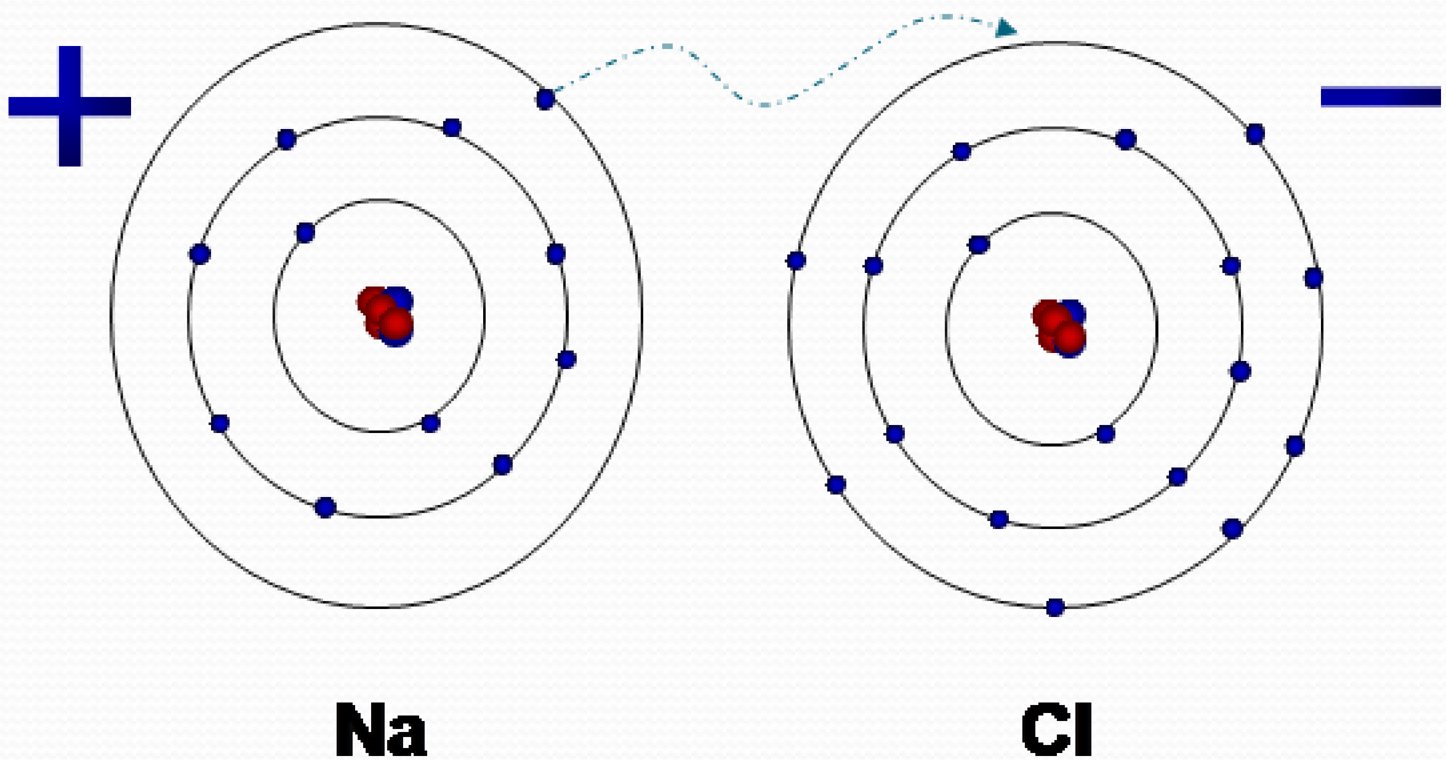
- All ionic compounds are crystalline solids at room temperature.

- NaCl is a typical example of ionic bonding.

Metallic elements have only up to the valence electrons in their outer shell.

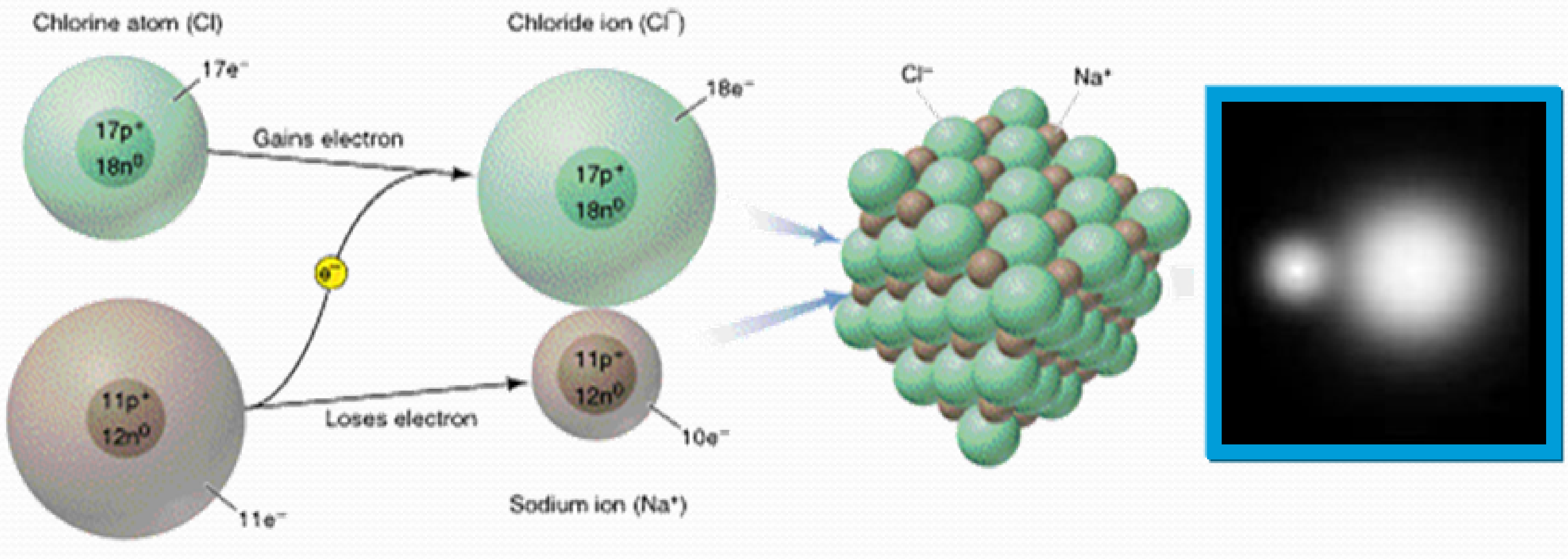
When losing their electrons they become positive ions.

Electronegative elements tend to acquire additional electrons to become negative ions or anions.

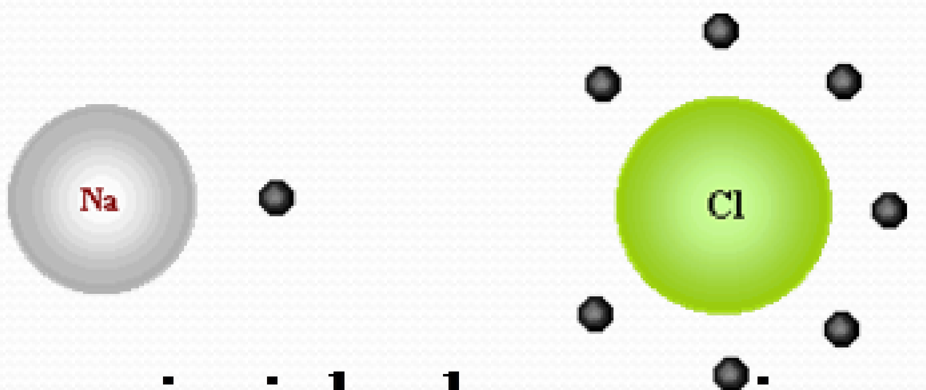


NaCl

- Notice that when sodium loses its one valence electron it gets smaller in size, while chlorine grows larger when it gains an additional valance electron. After the reaction takes place, the charged Na+ and Cl- ions are held together by electrostatic forces, thus forming an ionic bond.



- When the Na^+ and Cl^- ions approach each other closely enough so that the orbits of the electron in the ions begin to overlap with each other, then the electron begins to repel each other by virtue of the repulsive electrostatic coulomb force. Of course the closer together the ions are, the greater the repulsive force.



- Pauli exclusion principle has an important role in repulsive force. To prevent a violation of the exclusion principle, the potential energy of the system increases very rapidly.

Apabila ion Na^+ dan ion Cl berdekatan pada jarak r, besarnya energi (potensial) tarik-menarik Coulomb adalah :

$$E_{coul} = -e^2 / 4\pi \varepsilon_o r$$

energi tolak-menolak (repulsif) :

$$E_{rop} = A/r^n \quad \text{atau} \quad E_{rop} = B \exp(-r/\rho)$$

interaksi tolak-menolak berjangkauan pendek → setiap ion hanya "merasakan" interaksi tolak-menolak dengan ion tetangga terdekatnya saja.

Interaksi elektrostatik berjangkauan jauh → setiap ion akan berinteraksi baik dengan ion tetangga terdekatnya maupun dengan ion tetangga berikutnya

→ Energi Madelung

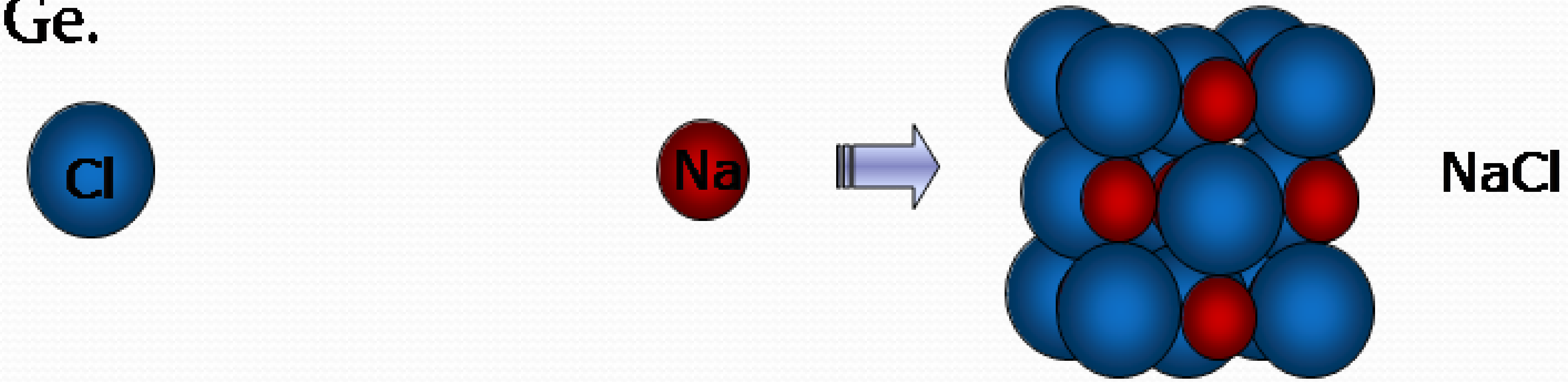
Beberapa **contoh** Kristal ionik

Kristal	r(nm)	Energi kohesif (eV)	n	Struktur
LiF	0,201	8,52	6	fcc
LiCl	0,257	6,85	7	fcc
NaCl	0,281	6,39	8	fcc
NaI	0,324	5,00	9,5	fcc
KCl	0,315	6,46	9	fcc
KBr	0,330	5,89	9,5	fcc
RbF	0,282	7,09	8,5	fcc
RbCl	0,329	6,34	9,5	fcc
CsCl	0,356	6,46	10,5	bcc
CsI	0,395	5, 35	12,0	bcc
MgO	0,210	9,34	7	fcc
BaO	0,275	8,90	9,5	fcc

Energies of Interactions Between Atoms

- The energy of the crystal is lower than that of the free atoms by an amount equal to the energy required to pull the crystal apart into a set of free atoms. This is called the binding (cohesive) energy of the crystal.

  - NaCl is more stable than a collection of free Na and Cl.
  - Ge crystal is more stable than a collection of free Ge.



Sifat kristal ionik

1. Keras dan stabil
2. Merupakan konduktor yang buruk, karena tidak ada elektron bebas
3. Suhu penguapannya tinggi sekitar 1000 sampai 2000 K
4. Tidak tembus cahaya
5. Mudah larut dalam cairan polar (air)
6. Menyerap radiasi infra merah

Ikatan Kovalen

Ikatan kovalen = *ikatan valensi atau homopolar* dibangun oleh sepasang elektron dari dua atom yang berikatan

Setiap atom ➔ satu elektron ➔ sebuah ikatan kovalen

Atom-atom yg berikatan kovalen menggunakan bersama sepasang elektron atau lebih

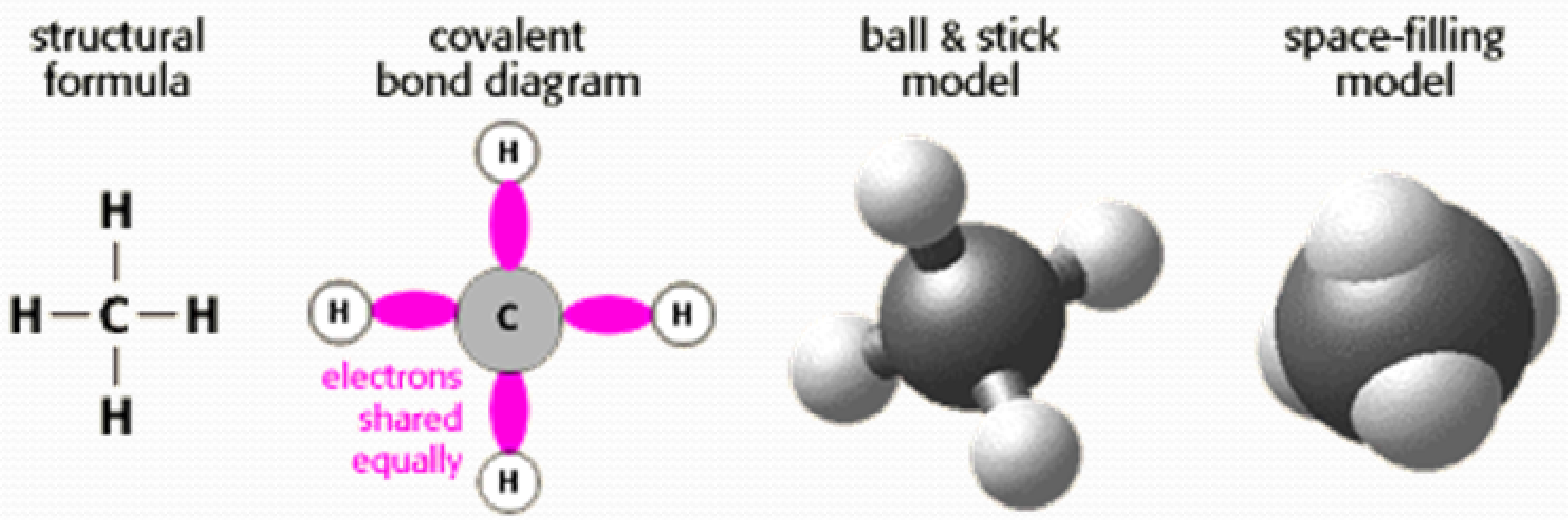
Ikatan kovalen ➔ kuat

COVALENT BONDING

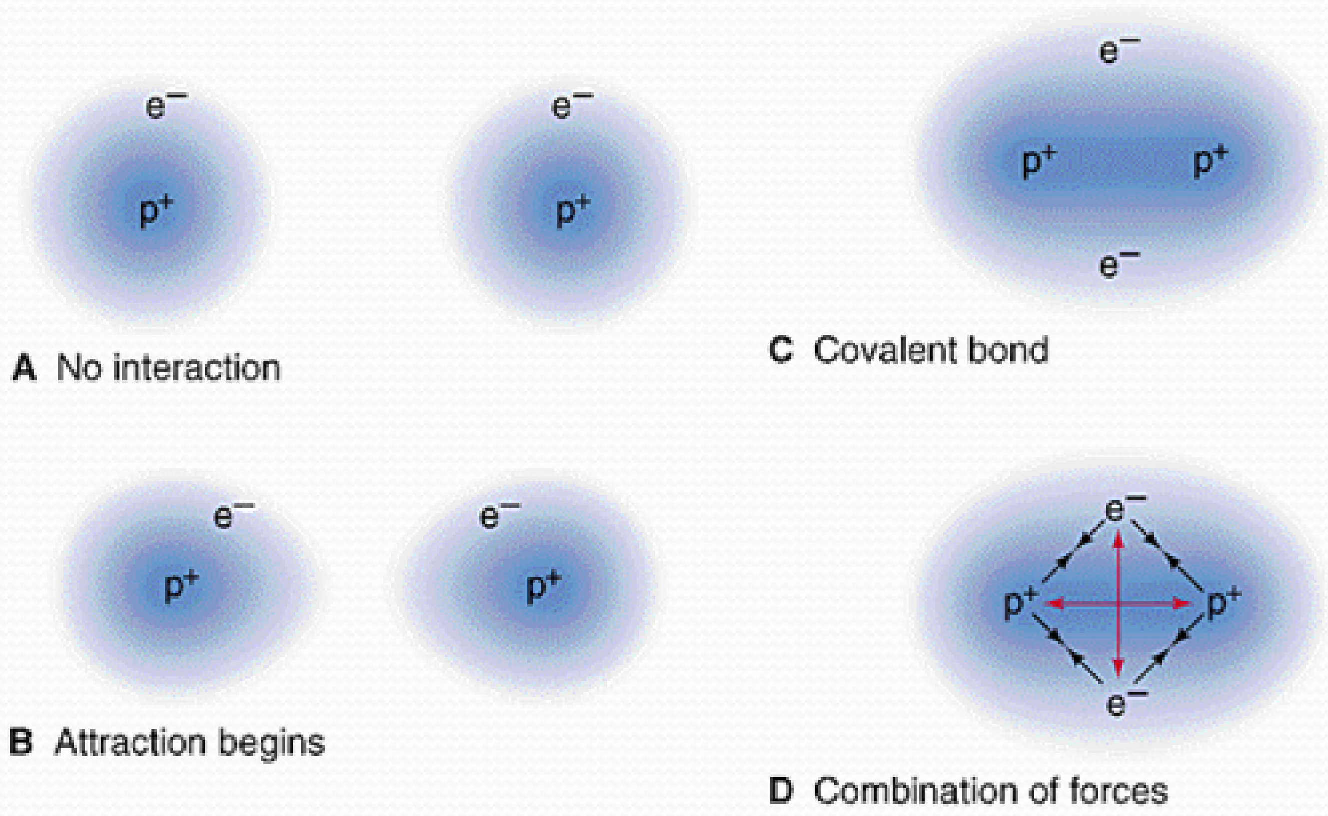
- Covalent bonding takes place between atoms with small differences in electronegativity which are close to each other in the periodic table (*between non-metals and non-metals*).

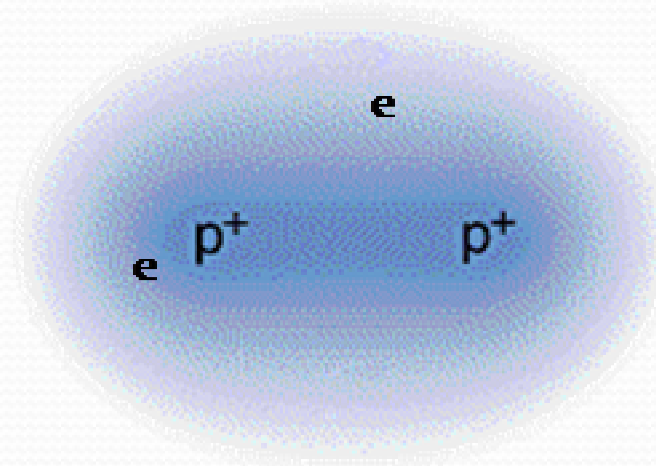
- The covalent bonding is formed when the atoms share the outer shell electrons (i.e., s and p electrons) rather than by electron transfer.

- Noble gas electron configuration can be attained.

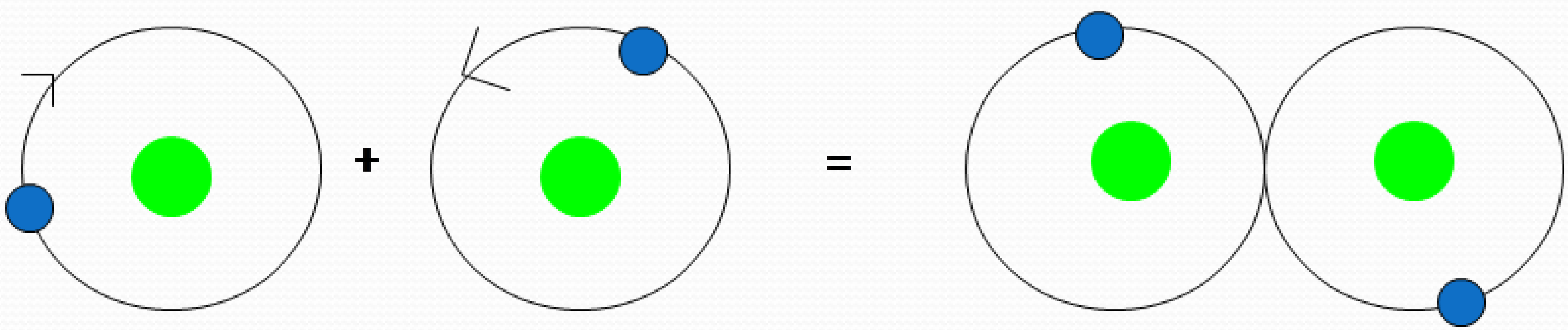


- Each electron in a shared pair is attracted to both nuclei involved in the bond. The approach, electron overlap, and attraction can be visualized as shown in the following figure representing the nuclei and electrons in a hydrogen molecule.





Atom hidrogen (H) memiliki konfigurasi $1s^1$,akan lebih stabil jika memakai bersama sepasang elektron dengan sebuah elektron hidrogen yang lain sehingga membentuk molekul H_2



H **H** **H_2**

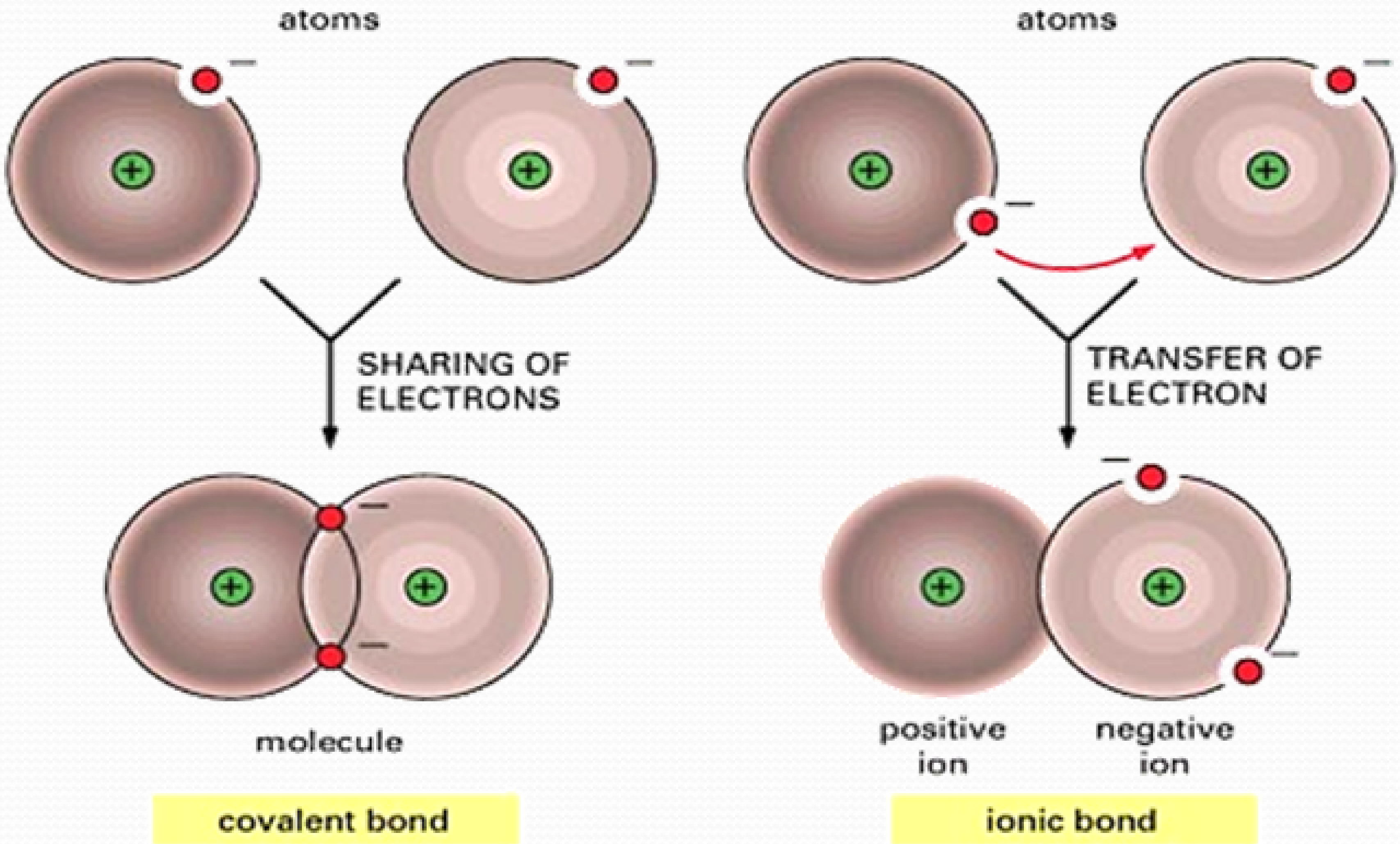
Beberapa contoh Kristal Kovalen

Kristal	r(nm)	Energi kohesif (eV)
ZnS	0,235	6,32
C(intan)	0,154	7,37
Si	0,234	4,63
Ge	0,244	3,85
Sn	0,280	3,14
CuCl	0,226	9,24
GaSb	0,265	6,02
InAs	0,262	5,70
SiC	0,189	12,3

Sifat-sifat Kristal kovalen

1. Tidak larut dalam zat cair biasa
2. Penghantar yang buruk
3. Tembus cahaya (contoh : intan)
4. Beberapa kristal kovalen sangat keras (intan, silikon karbid utk ampelas), karena energi kohesif kristal ini besar
5. Sebagian kristal, titik lelehnya sangat tinggi (intan = 4000 K)

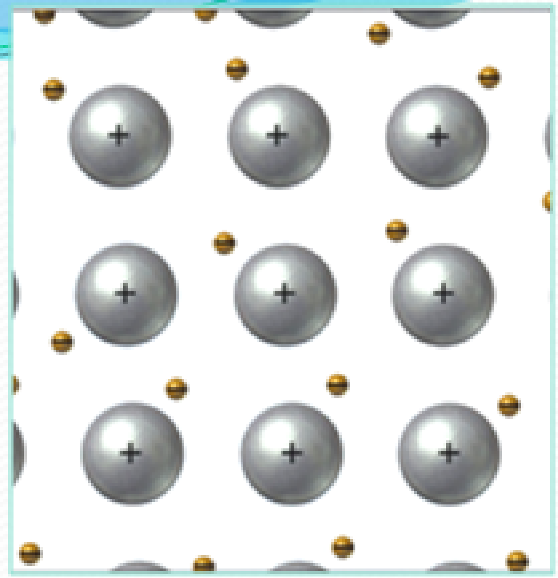
Comparison of Ionic and Covalent Bonding



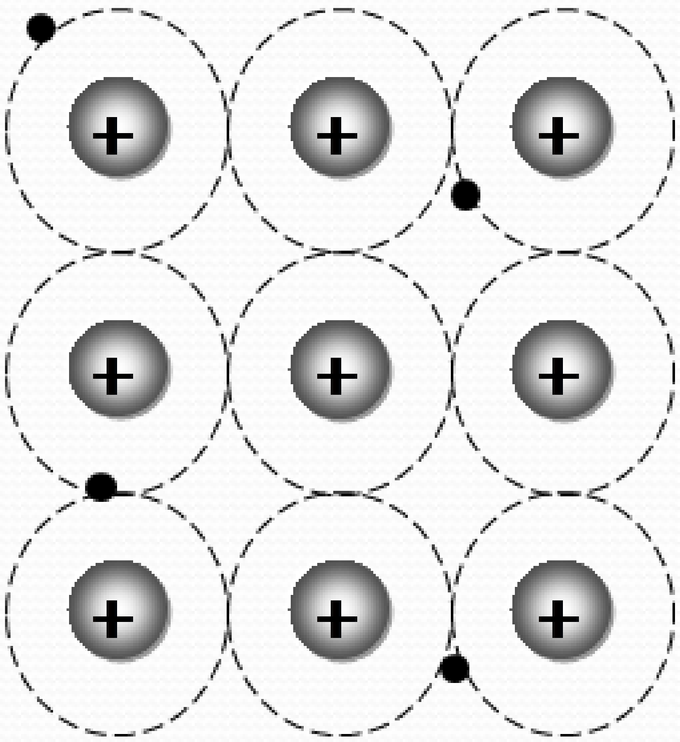
Ikatan Logam

- Setiap logam mempunyai elektron valensi (elektron terluar) yang sangat mudah bergerak.
- Elektron-elektron valensi dilukiskan sebagai *lautan awan/Gas* elektron yang membungkus ion-ion positif.
- Ikatan antara gas/awan elektron → *ikatan logam*.
- *Gas elektron* bertindak sbg "perekat" yang mengikat ion-ion positif utk membentuk suatu ***kristal logam***.
- Bentuk umum kristal logam adalah base center cubic (bcc) atau face center cubic (fcc). Sebagian berbentuk hexagonal close packed (hcp).

METALLIC BONDING



- Metallic bonding is found in metal elements. This is the electrostatic force of attraction between positively charged ions and delocalized outer electrons.
- The metallic bond is weaker than the ionic and the covalent bonds.
- A metal may be described as a low-density cloud of free electrons.
- Therefore, metals have high electrical and thermal conductivity.



What kind of forces hold the atoms together in a solid?

Apakah yang menyebabkan sebuah kristal tetap bersatu ?

- All valence electrons in a metal combine to form a “sea” of electrons that move freely between the atom cores. The more electrons, the stronger the attraction. This means the melting and boiling points are higher, and the metal is stronger and harder.
- The positively charged cores are held together by these negatively charged electrons.
- The free electrons act as the bond (or as a “glue”) between the positively charged ions.
- This type of bonding is nondirectional and is rather insensitive to structure.
- As a result we have a high ductility of metals - the “bonds” do not “break” when atoms are rearranged – metals can experience a significant degree of plastic deformation.

Beberapa contoh Kristal Logam

Logam	r(nm)	Energi kohesif (eV)	Struktur kristal
Fe	0,248	4,32	bcc
Li	0,304	1,66	bcc
Na	0,372	1,13	bcc
Cu	0,256	3,52	fcc
Ag	0,289	2,97	fcc
Pb	0,350	2,04	fcc
Co	0,251	4,43	Hcp(hexagonal close packed)
Zn	0,266	1,35	hcp
Cd	0,298	1,17	hcp

Sifat-sifat Kristal Logam

1. Tidak tembus cahaya
2. Permukaannya tampak mengkilap
3. Memiliki konduktivitas yang baik
4. Dapat dilarutkan dan dicampurkan dengan logam lain sehingga membentuk senyawa baru

Ikatan Hidrogen

Atom H hanya memiliki sebuah elektron ➔ atom hidrogen hanya dapat berikatan dengan sebuah atom lain.

Keadaan tertentu : atom hidrogen dapat pula berikatan cukup kuat dengan dua buah atom lain.

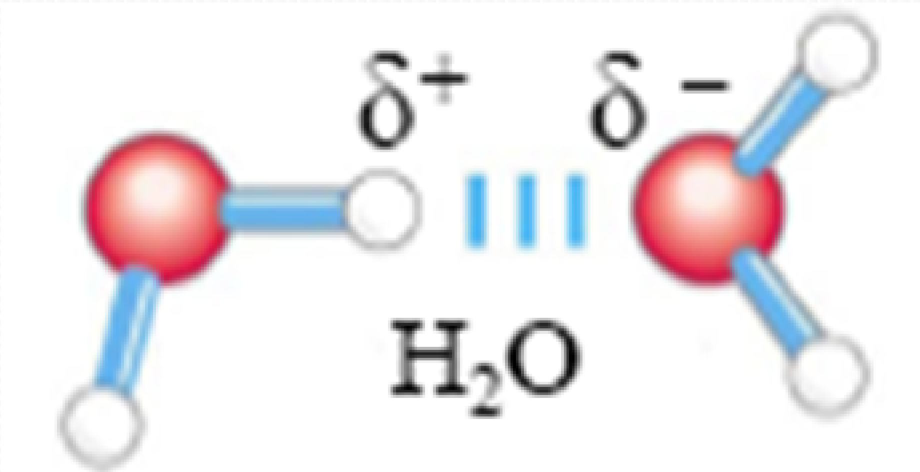
➔ Pada keadaan demikian terbentuklah ikatan hidrogen di antara atom-atom tersebut dengan atom H ➔ (energi ikat 0,1 eV.)

Dalam ikatan hidrogen, atom H bersifat sebagai ion positif terutama bila berikatan dengan atom-atom yang elektronegatif, seperti F, O dan N.

HYDROGEN BONDING

- A hydrogen atom, having one electron, can be covalently bonded to only one atom. However, the hydrogen atom can involve itself in an additional electrostatic bond with a second atom of highly electronegative character such as fluorine or oxygen. This second bond permits a ***hydrogen bond*** between two atoms or strucures.
- The strength of hydrogen bonding varies from 0.1 to 0.5 ev/atom.

- Hydrogen bonds connect water molecules in ordinary ice. Hydrogen bonding is also very important in proteins and nucleic acids and therefore in life processes.



Sifat-sifat ikatan Hidrogen

1. Wujud cair, ikatan hidrogen antara satu molekul H_2O dengan molekul H_2O yang lain mudah putus, akibat gerak termal atom-atom H dan O. Namun dapat tersambung dengan molekul H_2O yang letaknya relatif lebih jauh.
2. Wujud padat, ikatan hidrogennya lebih stabil karena energi termalnya lebih rendah dari energi ikat hidrogen : kristal es (suhunya lebih rendah)

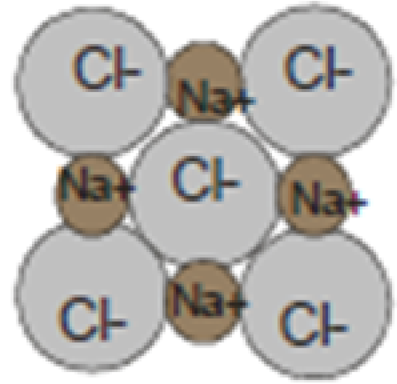
IKATAN PADA KRISTAL

Jenis Ikatan	Asal ikatan	Sifat
Kovalen	Patungan elektron	Sangat keras; titik lebur tinggi; larut dalam sedikit cairan; transparan terhadap cahaya tampak
Ionik	Gaya tarik menarik elektrostatik antara ion positif dan ioan negatif	Keras; titk lebur tinggi; larut dalam cairan polar seperti air
Hidrogen	Gaya tarik menarik elektrostatik kuat antara hidrogen pada satu molekul dengan atom N, O atau F	Lebih kuat dari ikatan Van der Wals, titik lebur dan titik didih lebih tinggi dari ikatan Van der Wals
Van der Waals	Gaya Van der Waals akibat distribusi muatan yang tidak simetris	Lunak; titik lebur dan titik didih rendah ; larut dalam cairan kovalen
Logam	Gaya tarik menarik elektrostatik antara ion positif logam dengan awan elektron	Berkilauan; menghantarkan kalor dan listrik dengan baik

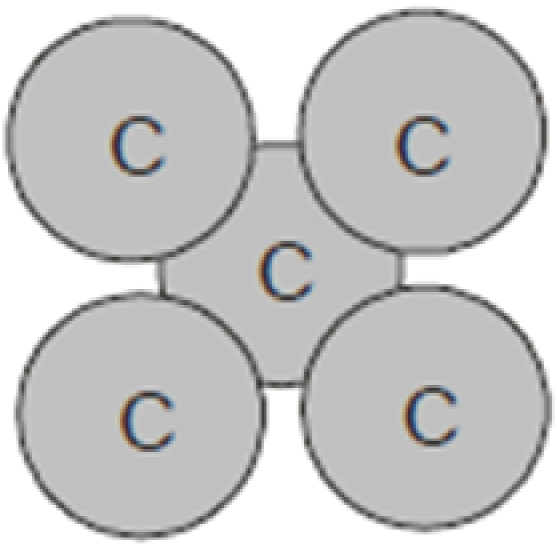
Types of Bonding

Ionic Bonding	Van Der Waals Bonding	Metallic Bonding	Covalent Bonding	Hydrogen Bonding
High Melting Point	Low Melting Points	Variable Melting Point	Very High Melting Point	Low Melting Points
Hard and Brittle	Soft and Brittle	Variable Hardness	Very Hard	Soft and Brittle
Non conducting solid	Non-Conducting	Conducting	Usually not Conducting	Usually Non-Conducting
NaCl, CsCl, ZnS	Ne, Ar, Kr and Xe	Fe, Cu, Ag	Diamond, Graphite	İce, organic solids

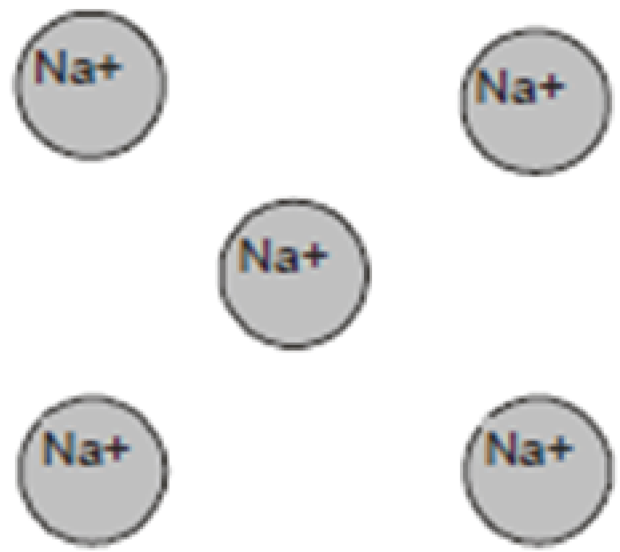
Crystalline-Argon
(van der waals)



Sodium Chloride
(ionic)



Diamond (covalent)



Sodium (metallic)

ENERGI IKAT

Gaya Ikat,Jarak Ikatan, dan Energi Ikat

Gaya Ikat → **adalah resultan dari gaya tarik elektrostatik (antar proton–elektron) dan gaya tolak elektrostatik (proton–proton)**

<u>Besar gaya tarik dan tolak :</u>

$r > r_o$ gaya tarik lebih besar

$r < r_o$ gaya tolak lebih besar

r = ∝c gaya tarik dan gaya tolak = 0

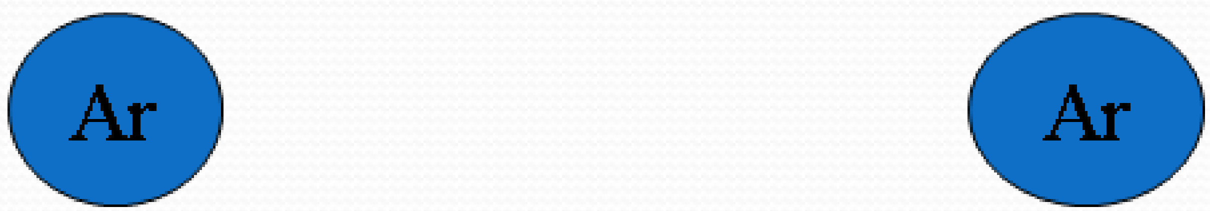
$r = r_o$ gaya tarik = gaya tolak, sehingga ro disebut jarak keseimbangan atau jarak ikatan

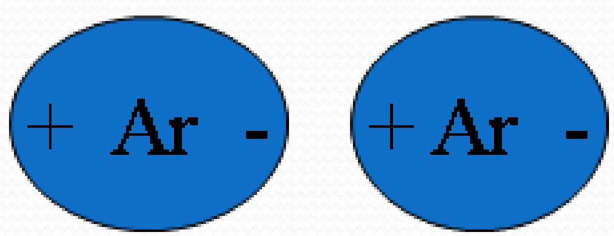
Gaya elektrostatik tarik-menarik antara muatan negatif elektron dan muatan positif inti atom → *gaya pemersatu (kohesi) dalam zat padat*

Interaksi pertukaran, sepeti gaya van der waals dan lkatan kovalen memberikan sumbangan yang berarti pada *kohesi* kristal.

Gaya magnet dan gaya gravitasi sangat kecil pengaruhnya pada kohesi → diabaikan efeknya.

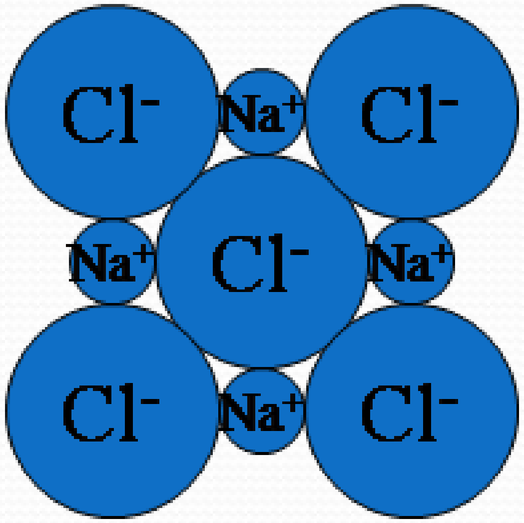
- Bonding energy: ~0.01 eV (weak)
- Compared to thermal vibration energy $k_B T$ ~ 0.026 eV at T = 300 K
- Examples: inert gases





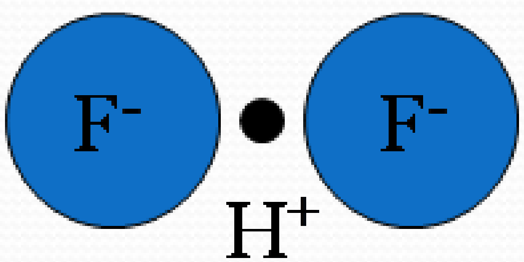
Dipole-dipole interaction

Ionic Bond



- The electron of the Na atom is removed and attached to the Cl atom
- Bonding energy: 1-10 eV (strong)

Hydrogen bond

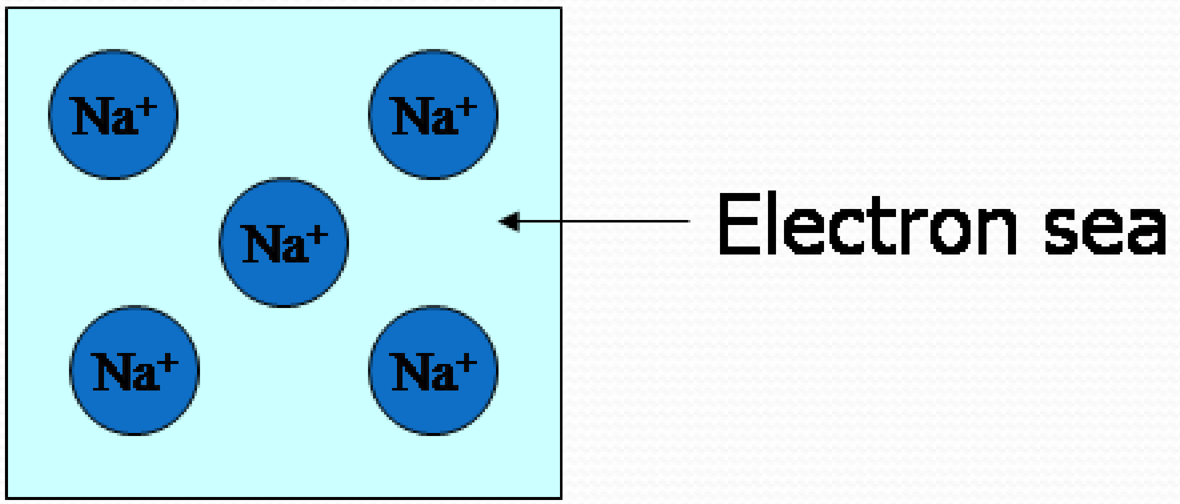


HF_2^- molecule

- The electron of the H atom is pulled toward the other atom
- Ionic in nature
- Bonding energy: ~k_BT (weak)
- Examples: DNA; intermolecular bond between water and ice

Metallic Bond

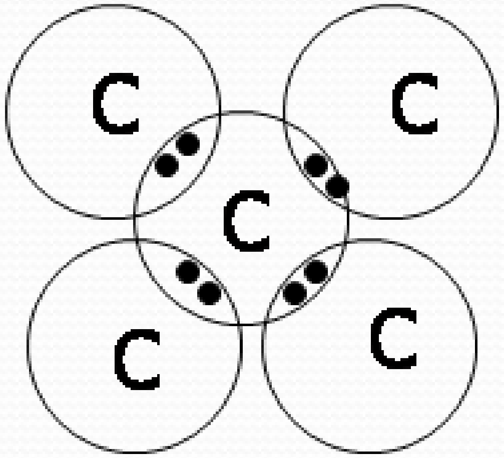
Positive ions in a sea of electrons



- Bonding energy:
  ~1-10 eV (strong)

Covalence bond

H• + •H → H:H



- Two atoms share a pair of electrons
- Bonding energy: ~1-10 eV (strong)
- Examples: C, Ge, Si, H_2

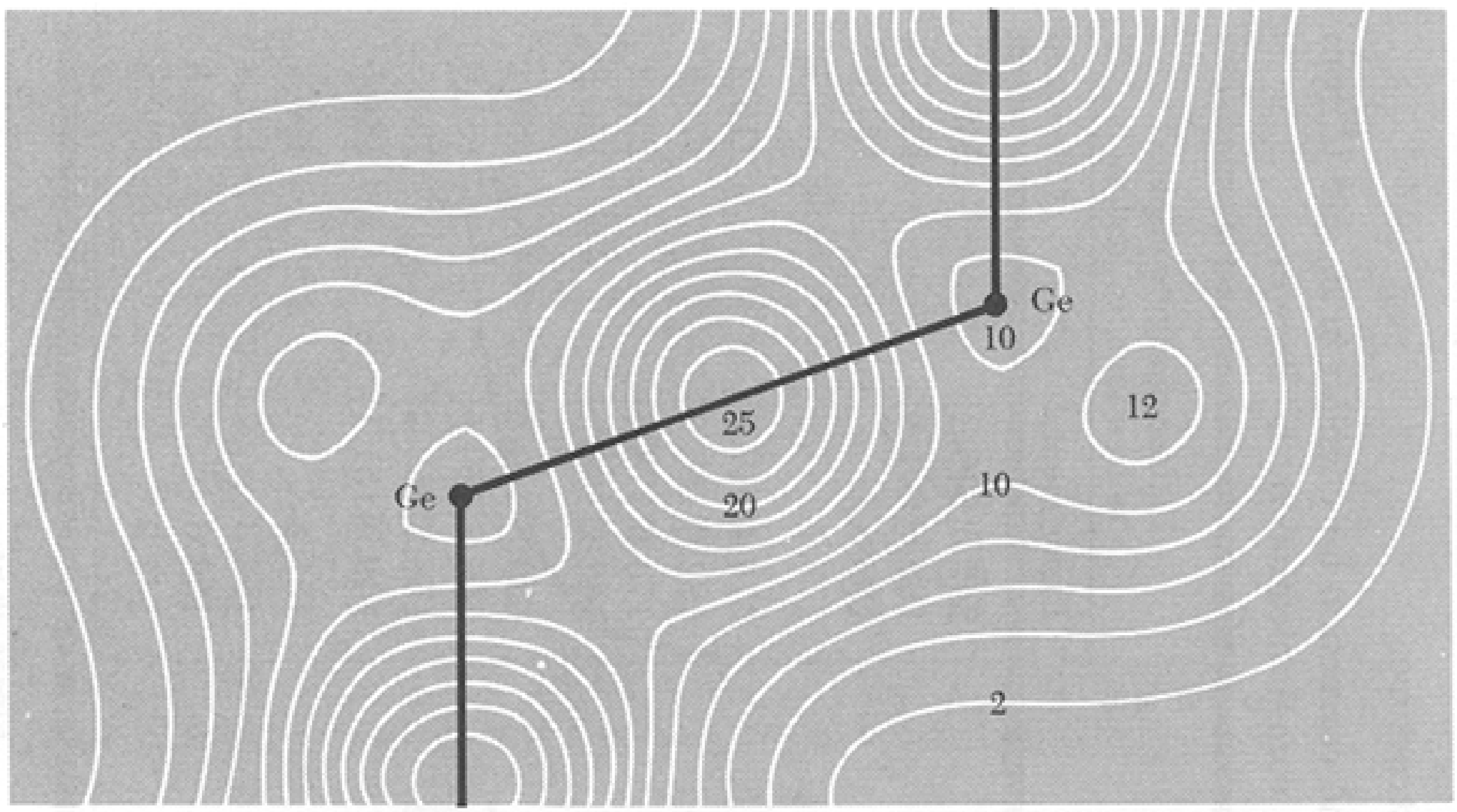
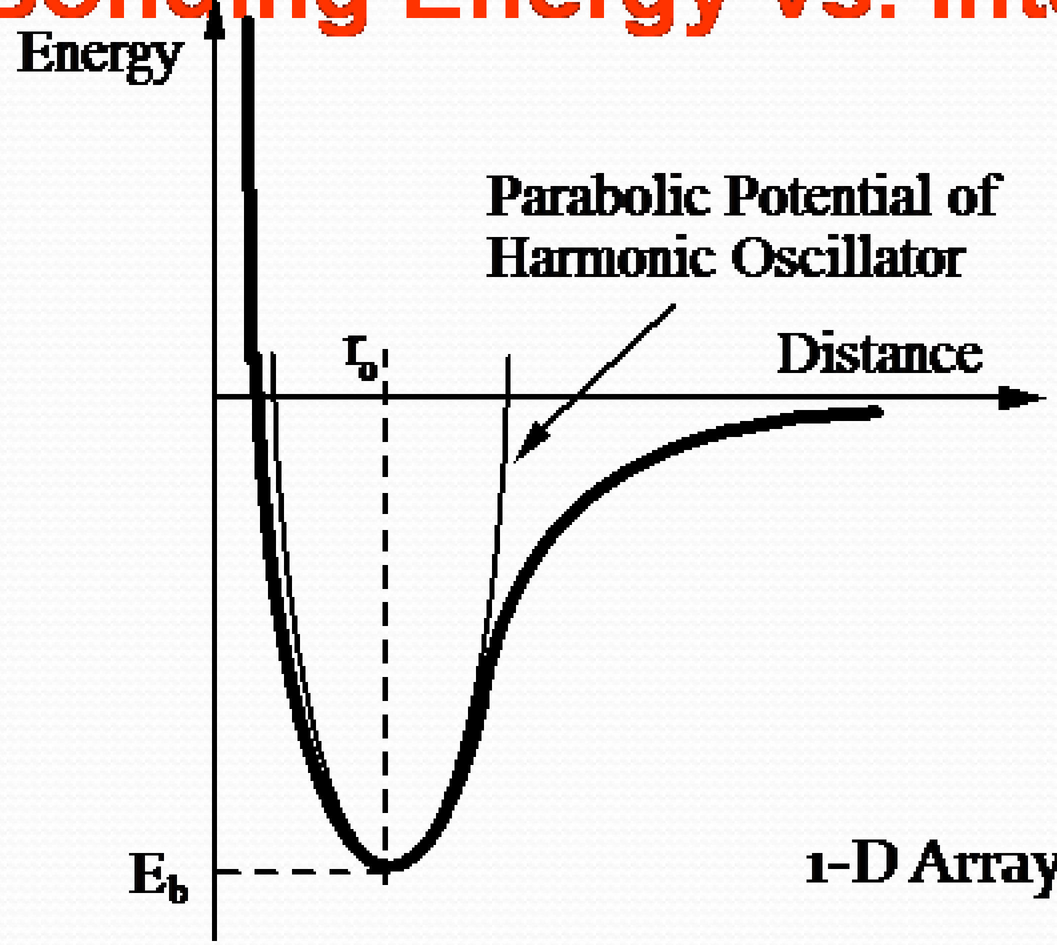
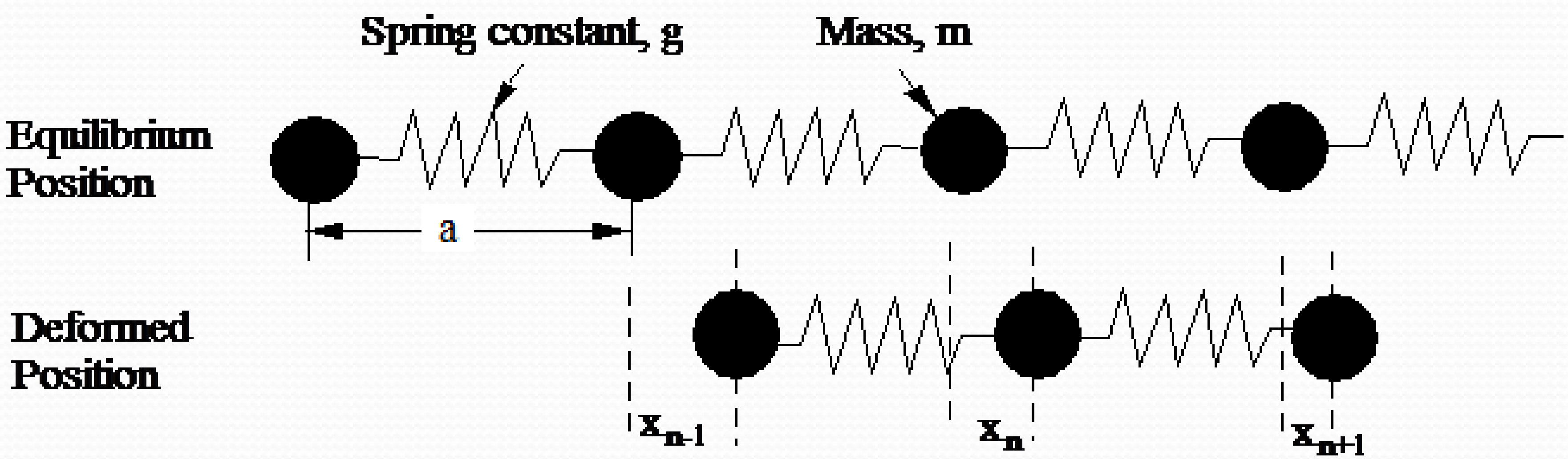


Figure 11 Calculated valence electron concentration in germanium. The numbers on the contours give the electron concentration per primitive cell, with four valence electrons per atom (eight electrons per primitive cell). Note the high concentration midway along the Ge-Ge bond, as we expect for covalent bonding. (After J. R. Chelikowsky and M. L. Cohen.)

Bonding Energy vs. Inter-atomic Distance



1-D Array of Spring Mass System



Energi kohesi dari sebuah kristal :
energi yang harus diberikan kepada kristal untuk memisahkan komponen-komponenya menjadi atom-atom bebas yang netral pada keadaan diam dan pada jarak tak hingga.

Untuk kristal yang bersifat ionik :
Energi kohesi = energi kisi (lattice energy)
➔ energi yang harus diberikan pada kristal untuk memisahkan komponen-komponennya menjadi ion-ion bebas pada keadaan diam dan pada jarak tak hingga.

Cara atom berikatan satu sama lain dalam membentuk kristal :

- Ikatan Van Der Waals
- Ikatan Ionik
- Ikatan Kovalen
- Ikatan Logam
- Ikatan Hidrogen

Types of Bonding Mechanisms

It is conventional to classify the bonds between atoms into different types as

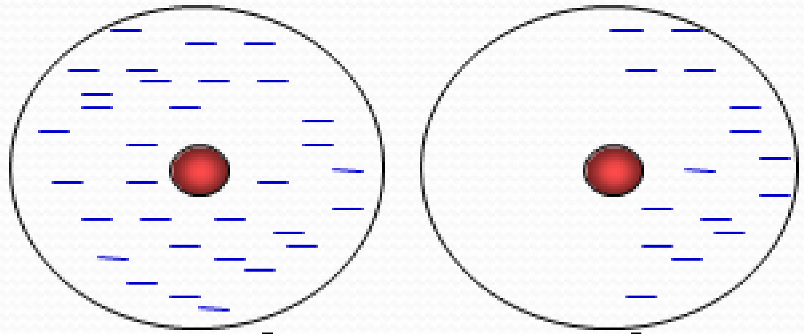
- Ionic
- Covalent
- Metallic
- Van der Waals
- Hydrogen

All bonding is a consequence of the electrostatic interaction between the nuclei and electrons.

Ikatan Van Der Waals

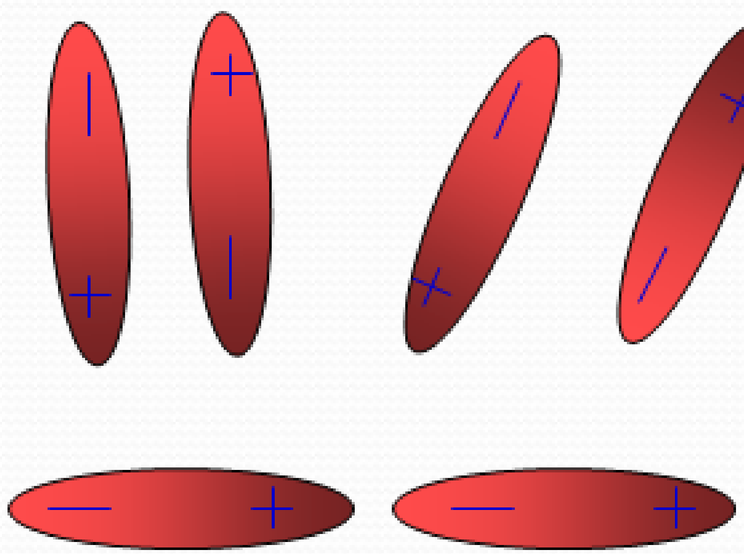
- Kristal pada golongan VIIIA (gas mulia) ➔ Ne, Ar, Kr, Xe, Rn.
- Atom-atom gas inert dapat mengalami *distorsi* yang sangat kecil pada distribusi elektronnya dalam orbital kulit penuh yang berbentuk simetri bola.
- Penyimpangan ini cukup mengubah atom-atom menjadi dipol-dipol listrik.
- Interaksi antar dipol inilah yang menghasilkan gaya tarik-menarik yang disebut gaya Van der Waals

The dipoles can be formed as a result of unbalanced distribution of electrons in asymettrical molecules. This is caused by the instantaneous location of a few more electrons on one side of the nucleus than on the other.

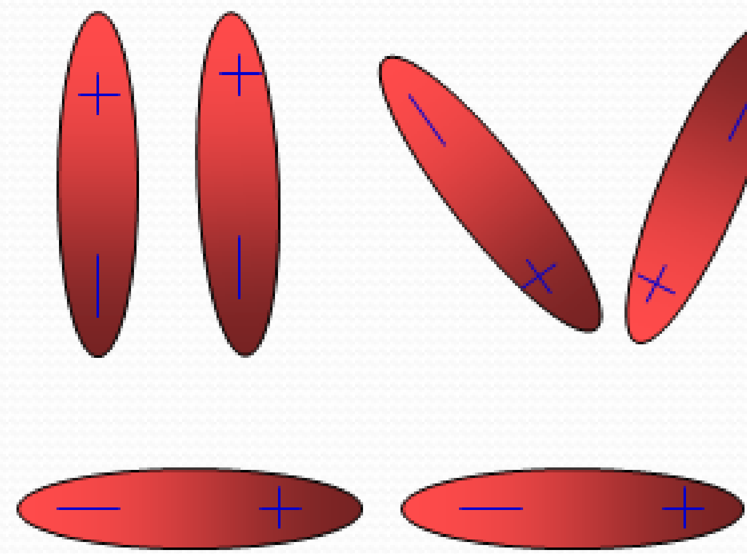


symmetric asymmetric

Therefore atoms or molecules containing dipoles are attracted to each other by electrostatic forces.



Display a marked attractive forces



No attraction is produced