Chapter 2 Atomic Structure and Interatomic Bonding

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1 Words

1. *vertical*
   垂直的
2. *van der Waals forces*
   范德华力
3. *adhesion*
   附着力
4. *adhesive*
   黏合剂
5. *incision*
   割口
6. *graphite*
   石墨
7. *hydrogen*
   氢
8. *constituent*
   组分
9. *uranium*
   铀
10. *isotope*
    同位素
11. *amu*
    原子质量单位
12. *crystalline*
    晶体的
13. *perpendicular*
    垂直的
14. *subshells*
    【核】支壳层
15. *overlap*
    交叠
16. *valence*
    【化】(化合)价；(原子)价
17. *neon*
    氖；氖气
18. *argon*
    氩
19. *krypton*
    氪
20. *helium*
    氦
21. *halogens*
    【化】卤(素)
22. *electronegative*
    负电性的
23. *shielded*
    屏蔽；保护
24. *insulators*
    绝缘物；绝热体
25. *adjacent*
    与…毗连的；邻近的
26. *infinite*
    极大的；无法衡量的；无限的
27. *versus*
    与；对
28. *gaseous*
    似气体的；含气体的

29. *prevail*
流行；盛行；战胜；压倒

30. *intermediate*
中间的

31. *slope*
斜坡；坡度

32. *dimensional*
尺寸的；空间的

33. *ionic*
离子的；电价的

34. *covalent*
共价的

35. *Ionic bonding*
离子键

36. *electronegativity*
电负性

37. *inasmuch*
由于

38. *brittle*
硬但易碎的；脆性的

39. *hybridization*
杂交；杂化

40. *symmetrically*
对称地

41. *molecules*
分子

42. *intramolecular*
作用于分子内的；存在于分子间的；发生于分子内的

43. *dipole*
偶极

44. *fluctuate*
波动

45. *predominate*
统治；居支配地位

46. *fluoride*
氟化物

47. *mayonnaise*
蛋黄酱

48. *anomalous*
异常的；反常的

49. *vertically*
垂直

2 Learning Objectives

1. ***Two atomic models:***

   (a) ***Bohr atomic model:***
   波尔原子模型
   In this model, electrons are assumed to revolve around the atomic nucleus in discrete orbitals, and the position of any particular electron is more or less well defined in terms of its orbital.
   在这种模型中，假设电子在原子核周围的离散轨道上旋转，并且任何特定电子的位置在其轨道中或多或少是明确的。

   (b) ***Wave-mechanical model:***
   波动力学模型
   In this model, the electron is considered to exhibit both wavelike and particle-like characteristics. With this model, an electron is no longer treated as a particle moving in a discrete orbital; rather, position is considered to be the probability of an electron being at various locations around the nucleus. In other words, position is described by a probability distribution or electron cloud.

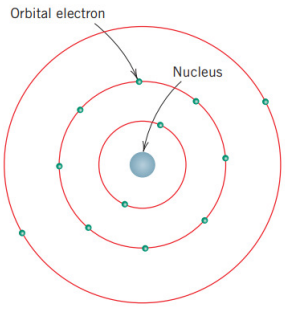

Figure 1: Schematic representation of the Bohr atom.

在这种模型中，电子被认为同时表现出波动性和粒子性特征。根据这种模型，电子不再被视为在离散轨道上运动的粒子；相反，位置被认为是电子在核周围不同位置出现的概率。换句话说，位置是通过概率分布或电子云来描述的。

Comparison

Both models are used widely, the choice depends on which model allows the simplest explanation.

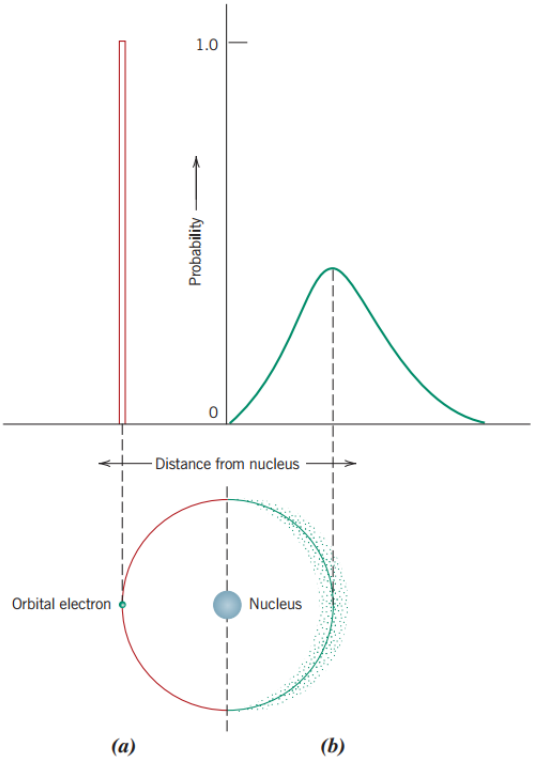

Figure 2: Comparison of the *(a)* Bohr and *(b)* wave-mechanical atom models in terms of electron distribution.

2. ***Quantum-mechanical principle that relates to electron energies:***
   与电子能量有关的量子力学原理
   One early outgrowth of quantum mechanics was the simplified Bohr atomic model, in which electrons are assumed to revolve around the atomic nucleus in discrete orbitals, and the position of any particular electron is more or less well defined in terms of its orbital.

量子力学的一个早期成果是简化的玻尔原子模型，在该模型中，电子被假设在离散的轨道上围绕原子核旋转，并且任何特定电子的位置可以通过其轨道或多或少地确定。

Another important quantum-mechanical principle stipulates that the energies of electrons are quantized-that is, electrons are permitted to have only specific values of energy. An electron may change energy, but in doing so, it must make a quantum jump either to an allowed higher energy (with absorption of energy) or to a lower energy (with emission of energy). Often, it is convenient to think of these allowed electron energies as being associated with energy levels or states. These states do not vary continuously with energy-that is, adjacent states are separated by finite energies. For example, allowed states for the Bohr hydrogen atom are represented in Figure 3(a). These energies are taken to be negative, whereas the zero reference is the unbound or free electron. Of course, the single electron associated with the hydrogen atom fills only one of these states.

另一个重要的量子力学原理规定，电子的能量是量子化的——也就是说，电子只能具有特定的能量值。电子可以改变能量，但在此过程中，它必须通过量子跃迁要么跃迁到允许的更高能量（吸收能量），要么跃迁到更低能量（释放能量）。通常，将这些允许的电子能量与能级或状态相关联是方便的。这些状态的能量并不是连续变化的——也就是说，相邻状态之间有有限的能量差。例如，玻尔氢原子的允许状态如图3(a)所示。这些能量被认为是负值，而零参考点是未绑定或自由电子。当然，与氢原子关联的单个电子仅填充其中一个状态。

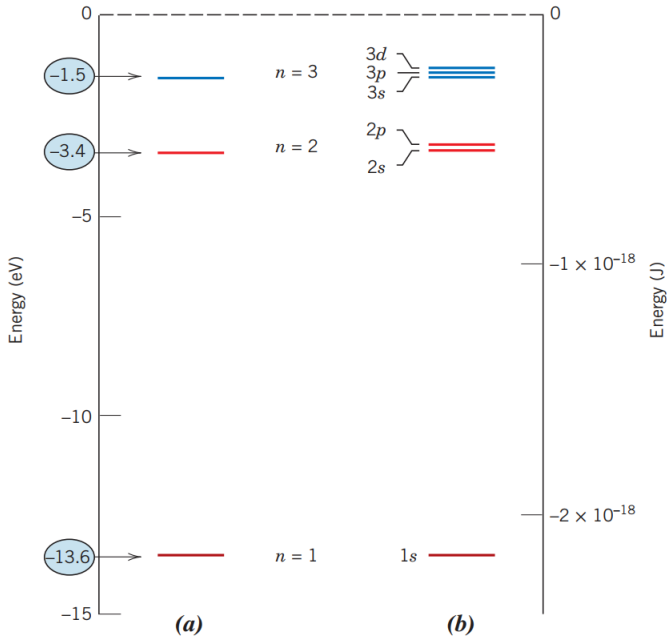

Figure 3: *(a)* The first three electron energy states for the Bohr hydrogen atom. *(b)* Electron energy states for the first three shells of the wave-mechanical hydrogen atom.

3. ***Boning forces and Energies:***

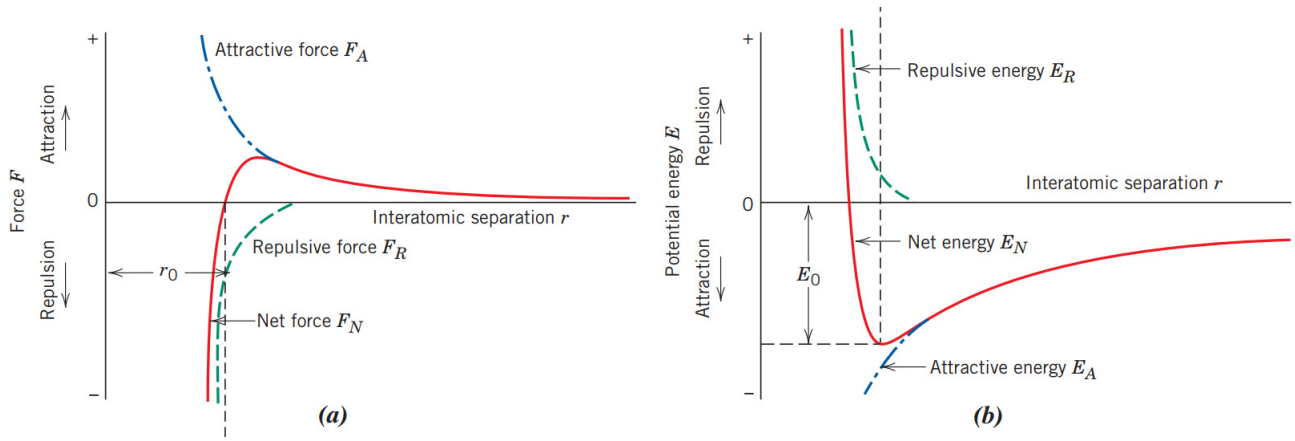

Figure 4: *(a)* The dependence of repulsive, attractive, and net forces on interatomic separation for two isolated atoms.*(b)* The dependence of repulsive, attractive, and net potential energies on interatomic separation for two isolated atoms.

4. ***Primary interatomic bonds:***

(a) ***ionic bonding:***

离子键

It is always found in compounds composed of both metallic and nonmetallic elements, elements situated at the horizontal extremities of the periodic table. Atoms of a metallic element easily give up their valence electrons to the nonmetallic atoms. In the process, all the atoms acquire stable or inert gas configurations (i.e., completely filled orbital shells) and, in addition, an electrical charge—that is, they become ions. Sodium chloride (NaCl) is the classic ionic material. A sodium atom can assume the electron structure of neon (and a net single positive charge with a reduction in size) by a transfer of its one valence 3s electron to a chlorine atom. After such a transfer, the chlorine ion acquires a net negative charge, an electron configuration identical to that of argon; it is also larger than the chlorine atom.

它总是存在于由金属和非金属元素组成的化合物中，这些元素位于周期表的水平两端。金属元素的原子容易将其价电子转移给非金属原子。在这个过程中，所有原子都获得了稳定的惰性气体电子配置（即完全填满的轨道壳层），并且带有电荷——也就是说，它们变成了离子。氯化钠（NaCl）是经典的离子材料。钠原子可以通过将其一个价电子（3s电子）转移给氯原子，从而获得与氖相同的电子结构，同时带有一个净正电荷并且体积减小。在这样的转移之后，氯离子获得了净负电荷，其电子配置与氩相同，同时其体积也大于氯原子。

(b) ***coulombic force:***

库仑力

Positive and negative ions, by virtue of their net electrical charge, attract one another.

正离子和负离子由于带有净电荷而互相吸引。

The attractive energy E_A:

$$E_A = -\frac{A}{r} \tag{1}$$

Theoretically, the constant A is equal to:

$$A = \frac{1}{4\pi\varepsilon_0}(|Z_1|e)(|Z_2|e) \tag{2}$$

Repulsive energy E_R:

$$E_R = \frac{B}{r^n} \tag{3}$$

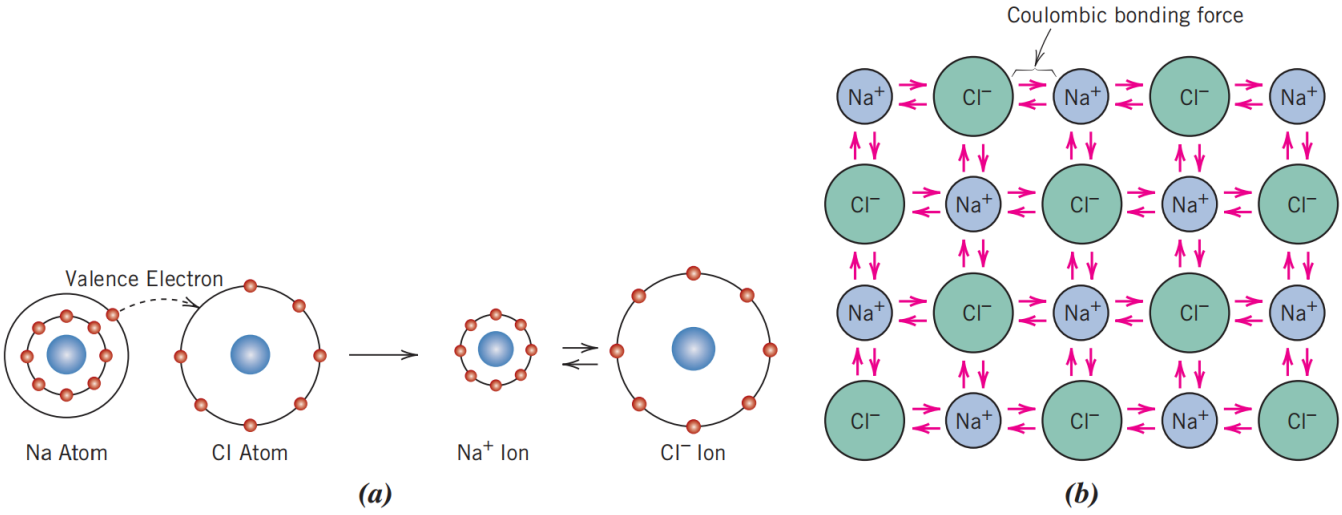

Figure 5: *(a)* The dependence of repulsive, attractive, and net forces on interatomic separation for two isolated atoms.*(b)* The dependence of repulsive, attractive, and net potential energies on interatomic separation for two isolated atoms.

(c) ***Covalent Bonding:***

共价键

Covalent bonding is found in materials whose atoms have small differences in electronegativity—that is, that lie near one another in the periodic table. For these materials, stable electron configurations are assumed by the sharing of electrons between adjacent atoms. Two covalently bonded atoms will each contribute at least one electron to the bond, and the shared electrons may be considered to belong to both atoms. Covalent bonding is schematically illustrated in Figure 2.12 for a molecule of hydrogen (H2). The hydrogen atom has a single 1s electron. Each of the atoms can acquire a helium electron configuration (two 1s valence electrons) when they share their single electron. Furthermore, there is an overlapping of electron orbitals in the region between the two bonding atoms. In addition, the covalent bond is directional—that is, it is between specific atoms and may exist only in the direction between one atom and another that participates in the electron sharing.

共价键存在于那些原子间电负性差异较小的材料中，也就是说，这些原子在周期表中相互接近。对于这些材料，稳定的电子配置通过相邻原子之间的电子共享来实现。两个共价键合的原子各自至少贡献一个电子给键，且共享的电子可以被视为属于两个原子。氢分子（H）的共价键在图2.12中进行了示意说明。氢原子有一个单独的1s电子。当两个原子共享各自的单个电子时，它们可以获得氦的电子配置（两个1s价电子）。此外，在两个键合原子之间的区域内，电子轨道会发生重叠。另外，共价键是有方向性的——也就是说，它存在于特定的原子之间，并且可能仅存在于参与电子共享的一个原子与另一个原子之间的方向上。

(d) ***Metallic Bonding:***

金属键

Metallic bonding is a type of chemical bonding that occurs in metals. In this bonding, metal atoms lose their outermost electrons, which become delocalized and free to move throughout the structure. This creates a "sea of electrons" that surrounds positively charged metal ions.

金属键是一种发生在金属中的化学键。在这种键合中，金属原子失去最外层的电子，这些电子变得离域化，并可以在整个结构中自由移动。这形成了一个“电子海”，环绕着带正电的金属离子。

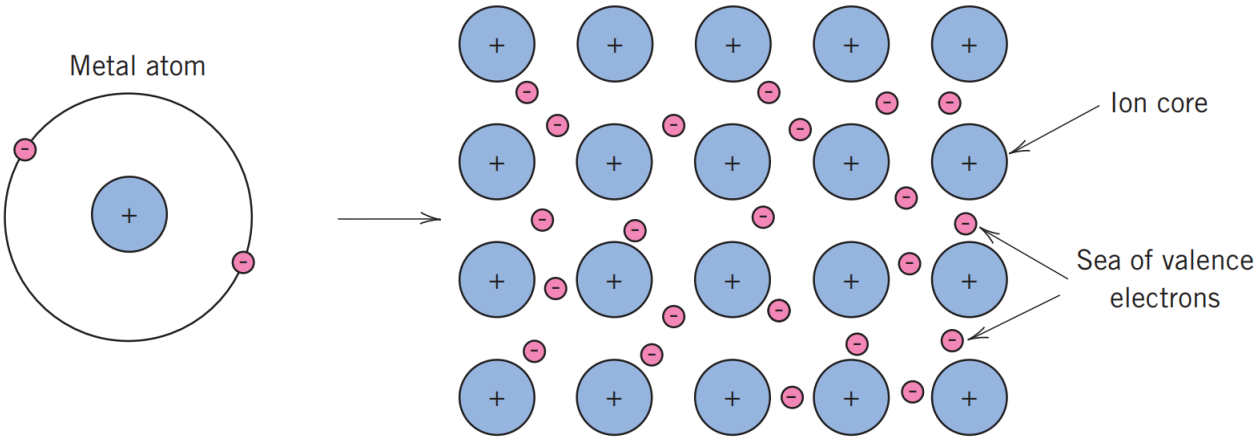

Figure 6: Schematic illustration of metallic bonding.

3 Summary

Why are the atomic weights of the elements generally not integers? Cite two reasons. *The atomic weights of elements are generally not integers due to two primary reasons:*

1. ***Isotopic Variation***
   Elements in nature are typically found as mixtures of isotopes, which are atoms of the same element with different numbers of neutrons. Each isotope has a slightly different mass due to the variation in the number of neutrons, and these masses are not whole numbers. The atomic weight of an element is an average of the masses of its isotopes, weighted by their relative abundance in nature. This averaging results in a non-integer value.
   自然界中的元素通常是同位素的混合物，即中子数不同的同种元素原子。由于中子数的不同，每种同位素的质量也略有不同，而且这些质量都不是整数。元素的原子量是其同位素质量的平均值，并根据它们在自然界中的相对丰度进行加权。这个平均值是一个非整数。

2. ***Mass Defect***
   The mass of an atom is slightly less than the sum of the masses of its individual protons, neutrons, and electrons due to the energy released when these particles combine to form the nucleus (as described by Einstein's equation $E = mc^2$). This difference in mass, known as the mass defect, accounts for the binding energy that holds the nucleus together. This effect contributes to the non-integer atomic weights observed in the periodic table.
   原子的质量略小于其单个质子、中子和电子的质量总和，这是由于这些粒子结合形成原子核时释放的能量（如爱因斯坦方程$E = mc^2$所述）。这种质量上的差异被称为质量缺陷，是将原子核固定在一起的结合能的原因。这种效应导致了元素周期表中观察到的非整数原子量。

4 Summary

1. ***Electrons in Atoms***

   - *The two atomic models are Bohr and wave mechanical. Whereas the Bohr model assumes electrons to be particles orbiting the nucleus in discrete paths, in wave mechanics we consider them to be wavelike and treat electron position in terms of a probability distribution.*

这两种原子模型是波尔模型和波动力学模型。波尔模型假设电子是以离散轨道围绕原子核旋转的粒子，而在波动力学中，我们认为电子具有波动性，并通过概率分布来描述电子的位置。

- *The energies of electrons are quantized—that is, only specific values of energy are allowed.*
  电子的能量是量子化的——也就是说，仅允许特定的能量值。

- *The four electron quantum numbers are n, l, m_l, and m_s. They specify, respectively, electron orbital size, orbital shape, number of electron orbitals, and spin moment.*
  四个电子量子数分别是 n、l、m_l和m_s。它们分别指定了电子轨道的大小、轨道的形状、电子轨道的数量以及自旋量子数。

- *According to the Pauli exclusion principle, each electron state can accommodate no more than two electrons, which must have opposite spins.*
  根据泡利不相容原理，每个电子态最多只能容纳两个电子，这两个电子必须具有相反的自旋。

2. ***The Periodic Table***
   元素周期表

   - *Elements in each of the columns (or groups) of the periodic table have distinctive electron configurations.*
     周期表中每一列（或组）的元素具有独特的电子配置。

3. ***Primary Interatomic Bonds***
   一次键

   - *For ionic bonds, electrically charged ions are formed by the transference of valence electrons from one atom type to another.*
     对于离子键，带电的离子是通过价电子从一种原子类型转移到另一种原子类型形成的。
     There is a sharing of valence electrons between adjacent atoms when bonding is covalent.
     当键合为共价键时，相邻原子之间会共享价电子。

   - *Electron orbitals for some covalent bonds may overlap or hybridize. Hybridization of s and p orbitals to form sp^3 and sp^2 orbitals in carbon was discussed. Configurations of these hybrid orbitals were also noted.*
     某些共价键的电子轨道可能会重叠或杂化。讨论了碳的s轨道和p轨道杂化以形成 sp^3 和 sp^2 轨道的情况，同时也提到了这些杂化轨道的构型。

   - *With metallic bonding, the valence electrons form a "sea of electrons" that is uniformly dispersed around the metal ion cores and acts as a form of glue for them.*
     在金属键中，价电子形成一个"电子海"，均匀地分布在金属离子核周围，充当将金属离子结合在一起的"粘合剂"。这种电子海模型解释了金属的导电性、延展性和光泽等特性。

4. ***Secondary Bonding or van der Waals Bonding***
   次键或范德华键

- *Relatively weak van der Waals bonds result from attractive forces between electric dipoles, which may be induced or permanent.*
  相对较弱的范德华键产生于电偶极子之间的吸引力，这种吸引力可能是诱导性的，也可能是永久性的。

- *For hydrogen bonding, highly polar molecules form when hydrogen covalently bonds to a nonmetallic element such as fluorine.*
  就氢键而言，当氢与氟等非金属元素共价结合时，就会形成高极性分子。

(a) ***Bonding TypeMaterial Classification Correlations***
键合类型与材料分类的相关性 Polymers—covalent
Metals—metallic
Ceramics—ionic/mixed ionic–covalent
Molecular solids—van der Waals
Semi-metals—mixed covalent–metallic
Intermetallics—mixed metallic–ionic

5. ***Equation Summary***

Table 1: ***Equation Summary***

Equation	***Solving For***
$E = \int F dr$	Potential energy between two atoms
$F = \frac{dE}{dr}$	Force between two atoms
$E_A = -\frac{A}{r}$	Attractive energy between two atoms
$E_R = \frac{B}{r^n}$	Repulsive energy between two atoms
$F_A = \frac{1}{4\pi\varepsilon_0 r^2}(\lvert Z_1\rvert e)(\lvert Z_2\rvert e)$	Force of attraction between two isolated ions
$\%\text{IC} = \{1 - \exp[-(0.25)(X_\text{A} - X_\text{B})^2]\} \times 100$	Percent ionic character

6. ***List of Symbols***

Table 2: ***List of Symbols***

Symbols	***Meaning***
A, B, n	Material constants
E	Potential energy between two atoms/ions
E_A	Attractive energy between two atoms/ions
E_R	Repulsive energy between two atoms/ions
e	Electronic charge
ε_0	Permittivity of a vacuum
F	Force between two atoms/ions
r	Separation distance between two atoms/ions
X_A	Electronegativity value of the more electronegative element for compound BA
X_B	Electronegativity value of the more electropositive element for compound BA
Z_1, Z_2	Valence values for ions 1 and 2