1 Introduction

Physics is the science of the structure and properties of inanimate matter. Molecular physics is the branch of physics concerned with the examination of the structure and properties of molecules using physical methods.

Lat. *moles* = mass, *molecula* = small mass

A molecule consists of two or more atoms, held together by a chemical bond. It is the smallest unit of a (non-atomic) chemical substance.

Binding energy (96 kJ per mol ≈ 1 eV per molecule):

- Chemical bonds: dissociation energy of 300 kJ mol^{-1} – 2000 kJ mol^{-1},
- Intermolecular interaction in liquids, molecular crystals, and molecules adsorbed at solid surfaces are in the order of magnitude of 50 kJ mol^{-1}. In gases, the interaction energy goes to zero as the pressure drops.

((Discussion of the figures given in the file freu_mol_intro.ppt))

The treating of problems in molecular physics is based on three pillars:

- The knowledge base of chemistry for interpreting chemical reactions, synthesis and analysis;
- The statements of quantum mechanics (quantum chemistry) for the explanation of molecular structures and properties;
- Physical measurement technology and methods.

This course is organized differently. Chapter 1 (Introduction) is followed by the chapters

2. Size, Mass and Kinetics of Molecules;
3. Molecules in Electric and Magnetic Fields;
4. Principles of Structure and Symmetry;
5. The Theory of Chemical Bonds;
6. Macromolecules;
7. Molecular Electronics;
8. Spectroscopy.

Thus, some basic theory is covered in chapters 3-5, the most important examination methods are described in chapters 2 and 8, and two examples of research areas in the field of molecular physics are treated in chapters 6 and 7. For the presentation of the most important spectroscopic methods that are integrated in this course Molecular Physics as Chapter 8 we will use some parts of another script which I use in the course "Spectroscopy for Physicists".

The course Molecular Physics put emphasis on the approaches of physicists to molecular problems. Molecular Physics is the consideration of the problems from the point of view of an experimental physicist. Other views to similar questions are chemistry, biology, material sciences and engineering including environmental engineering or environmental physics.

We could begin the history of molecular physics with Democritus [460-371 BC], who founded the atomic philosophy. This philosophy was later supported by Epicurius and Titus Carus Lucretius. Aristotle [384-322 BC] condemned it, however, and it remained unknown until the middle ages, when it was brought to light by Galileo Galilei [1564-1642]. An atomic concept of matter was supported by Robert Boyle, Isaac Newton and Christian Huygens, but opposed by Gottfried Wilhelm Leibniz. It was the basis for Daniel Bernoulli's kinetic theory of gases.

Quantitative considerations of chemical reaction led to John Dalton's law of constant and multiple proportions, which he wrote about in his book of 1808. In the same year, Louis Joseph Gay-Lussac found a relation of volumes in gas reactions which was unexplainable using Dalton's law.

A final solution was found in 1811 by the Italian physicist Avogadro [Lorenzo Romano Amedeo Carlo, Graf von Quaregna und Ceretto, 1776-1856]. His law states that the same volumes of ideal gases under the same pressure and at the same temperature have the same number of atomic groups, which he called "molecula". With that he founded an important basis for atomic and molecular physics, which needed another half century until its general acceptance.

To his honour, the number of molecules in a mole is called Avogadro's number. This number was first determined by Joseph Loschmidt in 1865 and is

$L = N_A = 6{,}0221367\ (36) \times 10^{23}\ \mathrm{mol}^{-1}$.

When Loschmidt first approximated this number, he also approximated the radius of a molecule.

It should be noted here that we use in this and other lecture scripts a comma as the decimal sign between digits in the numbers in agreement with ISO 31-0.

An exact understanding of chemical bonds has become possible with the advances in atomic and quantum physics. In 1915, the physicist Walter (Ludwig Julius Paschen Heinrich) Kossel developed an electrostatic model of the heteropolar chemical bond (ionic bond). He recognized the electronegativity of atoms as the source of the polarity of the bonding. The physical chemist Gilbert Newton Lewis published a paper in 1916 concerning the chemical homopolar bond caused by the creation of an electron pair. This was the fundament of the acid-base theory established in 1938/39.

Since 1927, the physicists Friedrich Hund, Walter Heinrich Heitler, and Fritz Wolfgang London laid important foundations of the quantum theory of chemical bonds, which has now become known as quantum chemistry.

Literature for the course Molecular Physics

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