Week 7 Chemistry in cyberspace

A. Listen to an interview and explain

- *the "shift of balance" between theoreticians and experimentalists in the chemical sciences*
- *the idea of a marriage between quantum physics and classical physics*
- *the comparison between chemical reactions and drama*

  (http://www.nobelprize.org/mediaplayer/index.php?id=1957)

B. Read the following text and answer the questions below.

Taking the experiment to cyberspace

Chemical reactions occur at lightning speed; electrons jump between atomic nuclei, hidden from the prying eyes of scientists. The Nobel Laureates in Chemistry 2013 have made it possible to map the mysterious ways of chemistry by using computers. Detailed knowledge of chemical processes makes it possible to optimize catalysts, drugs and solar cells. Chemists all over the world devise and carry out experiments on their computers on a daily basis. With the help of the methods that Martin Karplus, Michael Levitt and Arieh Warshel began to develop in the 1970s, they examined every tiny little step in complex chemical processes that are invisible to the naked eye.

Combining the best of both worlds

Previously when scientists wanted to simulate molecules on computers, they had software at their disposal that was based upon either classical Newtonian physical theories or quantum physics. Both had their strengths and weaknesses. The classical programs could calculate and process large chemical molecules. They would only display molecules in a state of rest, but gave chemists a good representation of how the atoms were positioned in the molecules. However, you could not use these programs to simulate chemical reactions. During the reaction, the molecules are filled with energy; they become excited. Classical physics simply have no understanding for such states, and that is a severe limitation.

When scientists wanted to simulate chemical reactions, they had to turn to quantum physics; the dualistic theory where electrons can be both particles and waves simultaneously. The strength of quantum physics is that it is unbiased and the model will not include any of the scientist's preconceptions. Therefore such simulations are more realistic. The downside is that these calculations require enormous computing power. The computer has to process every single electron and every atomic nucleus in the molecule. This can be compared to the number of pixels in a digital image. Many pixels will give you a high resolution, but also require more computer resources. Similarly, quantum physical calculations yield detailed descriptions of chemical processes, but require powerful computers. In the 1970s, this meant that scientists could only perform calculations on small molecules. When modelling, they were also forced to ignore interactions with the surrounding environment, although chemical reactions in real life most often occur in some kind of solution. However, if scientists would have wanted the computer to include the solvent in the calculation, they would have had to wait decades for the results.

So, classical and quantum chemistry were two fundamentally different, and in some respects rivalling, worlds. But the Nobel Laureates in Chemistry 2013 have opened a gate between these two worlds.

Focusing on the heart of the action

When chemists model chemical processes today, they apply the power where it is needed. They perform demanding quantum physical calculations on the very electrons and atomic nuclei that directly impact the chemical process. In that way, they get the best possible resolution where it matters. The other parts of the molecules are modelled using classical equations.

In order not to waste computing power, Michael Levitt and Arieh Warshel have trimmed the calculation workload even further. The computer does not always have to account for every single atom in the less interesting parts of the molecule. They have shown that it is possible to merge several atoms during the calculations.

In modern calculations, scientists also add a third layer to the simulation. Put in a somewhat simplified manner, the computer can, for areas very far away from the chemical process, bundle atoms and molecules into a single homogenous mass. In the scientific community this is referred to as dielectric medium.

How far the simulations will take us is for the future to decide

The fact that scientists these days can use computers to carry out experiments has yielded a much deeper understanding of how chemical processes work. The strength of the methods that Martin Karplus, Michael Levitt and Arieh Warshel have developed is that they are universal. They can be used to study all kinds of chemistry; from the molecules of life to industrial chemical processes. Scientists can optimize solar cells, catalysts in motor vehicles or even drugs, to take but a few examples. Progress will not stop there, however. In one of his publications, Michael Levitt writes about one of his dreams: to simulate a living organism on a molecular level. It is a tantalizing thought. The computer models that have been developed by the Nobel Laureates in Chemistry 2013 are powerful tools. Exactly how far they can advance our knowledge is for the future to decide.

(Adapted and abbreviated from: http://www.nobelprize.org/nobel_prizes/chemistry/laureates/2013/popular-chemistryprize2013.pdf)

1. ***Generally speaking, what is the main contribution of the 2013 Nobel Prize Laureates in Chemistry?***

   ____

2. ***In the past, what were simulations of large molecules based on?***

   ____

3. ***What were the main pluses and minuses of those simulations?***

   ____

4. ***What makes simulations of chemical reactions more authentic***?

   ____

5. ***What is the weakness of utilising quantum physics for simulating chemical reactions?***

   ____

6. ***Nowadays, simulation of chemical reactions is focused. In what sense?***

   ____

7. ***What are the main advantages of The Nobel Prize Laureates' methods?***

   ____

8. ***What is the vision of the future?***

   ____

C. *Find synonyms for the following expressions. The synonyms occur in the text.*

Example: every day __ ***on a daily basis*** ____

1) formed of parts or elements that are all of the same kind ________________________________
2) not observable without special devices ________________________________
3) they have the freedom to use it ________________________________
4) to make as perfect as possible ________________________________
5) happening or existing at the same time ________________________________
6) a substance that initiates/ accelerates a chemical reaction without itself being affected ________________________________
7) competing ________________________________
8) neighbouring, encircling ________________________________
9) fair, impartial, having no prejudice ________________________________
10) made easier to understand ________________________________

D. *Grammar and vocabulary: word formation*

1. Combine the words in brackets with suitable SUFFIXES to complete the sentences. Choose from the following suffixes:

-er, -or, -ing, -ion, -ness, -ity

1. A __________________ (boil) is a closed vessel in which water or other fluid is heated.
2. ________________ (compress) is the reduction in size of data in order to save space or transmission time.
3. In chemistry, the ____________________(dense) of many substances is compared to the______________ (dense) of water.
4. _______________________(transmit) is the act of passing something on.
5. _________________ (hard) is the characteristic of a solid material expressing its resistance to permanent deformation.
6. Combustion process is also called __________________ (heat).

-ify, -ise/-ize

1. I think this plan is too complicated. You should __________ (simple) it.
2. There used to be some disputes between the 2 countries but recently they have managed to _______________ (normal) their relations.
3. I hope you ________________ (real) that you are wrong.
4. When a liquid substance becomes solid, it ______________ (solid).

2. Match the following PREFIXES with their meanings.

bi-, mono-, multi-, poly-, dis-, in-, mal-, un-, de-, over-, ultra-, super-, re-, mis-

<u>number:</u>

<u>degree or size:</u>

<u>negativeness:</u>

<u>reverse:</u>

<u>repetition:</u>

Now match the following words with appropriate prefixes. Some words can be combined with several prefixes.

_____lingual	_____expected	_____atomic	_____compose
_____advantage	_____function	_____hydrate	_____violet

_____accuracy	_____cellular	_____frost	_____live
_____understand	_____charge	_____flow	_____take
_____open			

Explain the meaning of these expressions:

Understatement *Hypertext*

Hypertension *Subnormal*

Submerge *Supersonic*

*(Grammar and vocabulary exercises are based on **Velebná, English for chemists**)*