Computer-based molecular modelling: towards deeper understanding of chemistry

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Abstract: Models and modelling are essential factors in chemical thinking and in the development of scientific knowledge, therefore they should also be included in chemical education. This article illustrates the possibilities of computer-assisted molecular modelling in supporting chemistry teaching and learning. It justifies the need for molecular modelling and highlights the benefits of molecular modelling for both the teacher and the student.

Keywords: computer, molecular modelling, visualization

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1 Introduction

Chemical concepts are abstract by nature and therefore challenging to illustrate in an understandable way. The triple mode of representation brings more challenge to chemistry learning on the macro level, the sub-microscopic level and the symbolic level (Johnstone, 1993). At the macro level one can see and observe chemical phenomena. The sub-microscopic level justifies and illustrates the visible properties of a substance with atoms, molecules and ions (for example with molecular modelling). The symbolic level shows the macro level and micro level phenomena using chemical symbols, formulas and equations. It is important that teachers understand the threefold relationship so that it can be conveyed to their students (Gabel, 1999). While a teacher moves smoothly from one level to another, a student might be confused and get a fragmented vision of chemistry.

According to Gabel (1999), the primary barrier in understanding chemistry is that chemistry instruction occurs predominantly on the most abstract level, the symbolic level. The unobservable sub-microscopic level, in which phenomena and concepts are difficult to be combined with the students' perceptions and the living environment, produces also problems for students (Hinton & Nakhleh, 1999). Therefore, students need to use different models, analogies or computer graphics to make invisible into visible (Barnea, 2000).

Models and visualisation

Since models and modelling are essential in chemical thinking and in the development of scientific knowledge they should also be included in chemical education. Students should: learn about the nature of models and their usage as thinking tools; learn about the scope and the limitations of specific chemical models; be encouraged to use multiple models for a given phenomenon (Justi & Gilbert, 2002).

Visualizations help students to build mental models when learning about difficult concepts and sub-microscopic level phenomena. That is why the students' visualisation skills, spatial ability particularly, should be developed. Computer-based molecular modelling has helped a variety of learners to improve their visualisation skills and helped them to understand the concept of the model, three-dimensional molecular structure and chemical bonds (Barnea, 2000).

Computer-based molecular modelling

A molecular modelling software and computer-assisted learning materials enable new learning environments where chemistry concepts and phenomena can be viewed and perceived in a new manner. At the same time computer-assisted methods create new approaches enabling challenging chemistry topics to be clarified and simplified. Virtual models and visualisations can be modified according to the needs of teaching and learning (Jalonen, Lundell & Aksela, 2007).

Computer-based molecular modelling provides a tool for teaching and learning in order to support the visualisation of chemical phenomena and the development of chemistry teaching (Barnea & Dori, 1996; Lundell & Aksela, 2003; Jalonen et al., 2007; Pernaa, Aksela, & Lundell 2009; Dori & Kaberman, 2012). The computer enables to perceive things through visual experience which helps memorise things and improves learning outcomes (Lundell & Aksela, 2003). According to the experiences of Finnish school teachers, computer-based molecular modelling helps teachers to illustrate and students to learn difficult concepts in chemistry in a new way, it develops students' visualisation skills and makes students interested in chemistry (Aksela & Lundell, 2008). Finnish school teachers have used molecular modelling to illustrate the spatial structure of molecules, isomerism, atomic and molecular orbitals, chemical bonds, electron density, IR-spectroscopy, energy and its changes in chemical processes and chemical reactions. Molecular modelling can also be applied to biochemistry, biology and biotechnology education. According to Pernaa, Aksela and Lundell (2009), high school teachers experienced that molecular modelling supports the drawing of conclusions and the understanding of three-dimensional structures and it provides added value for teaching of orbitals, chemical bonds and biomolecules.

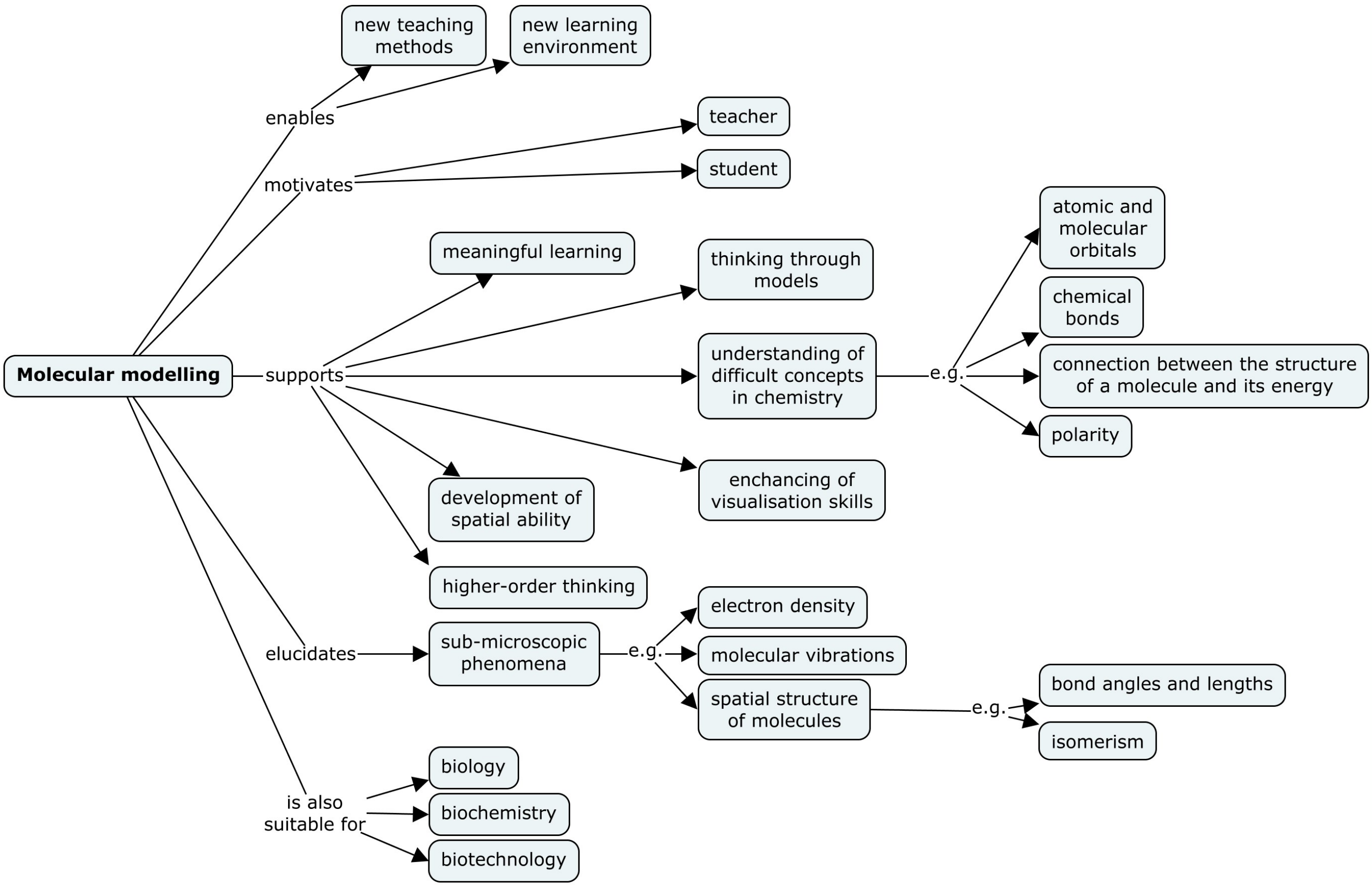

Figure 1. The possibilities of computer-based molecular modelling in chemistry teaching and learning.

Teachers and students generally have positive attitudes towards molecular modelling (Barnea & Dori, 1996; Aksela & Lundell, 2008). The teacher has an important role in the success and effectiveness of teaching chemistry through computer-based molecular modelling, because the use of modelling programs should not remain merely as a funny trick, instead working with a computer should be tied into teaching. The instructions and questions direct the learner's interest and activities in order to support learning tasks as well as it is possible and to train higher-order thinking skills (Aksela & Lundell, 2007).

The current learning theories highlight learning as a socially interactive process based on the students' experiences. By using computer-based molecular modelling it is possible to support the understanding of scientific concepts, practice different learning skills and to motivate students to investigate in an authentic research environment (Lundell & Aksela, 2003).

Software

There are multiple molecular modelling software options available for chemistry education – for molecular modelling Spartan (www.wavefun.com) and Avogadro (https://avogadro.cc); for chemical drawing ChemSketch (www.acdlabs.com) and MarvinSketch (www.chemaxon.com); and for web-based visualization e.g. Edumol (www.edumol.fi).

Conclusions

Upper secondary school students' thinking and conceptions about computer-based molecular modelling have been studied just a little. Findings indicate that molecular modelling has helped students to understand concepts in molecular geometry and bonding (Barnea & Dori, 1996) as well as in model concept, isomerism and functional groups (Dori & Barak, 2001). In the ongoing doctoral study, the meaningful teaching model for covalent bonds (as opposed to rote learning) is being developed. In this study, virtual models are also being developed and their effectiveness is researched on the students' learning of covalent bond and on the students' deeper understanding of chemistry (Figure 2).

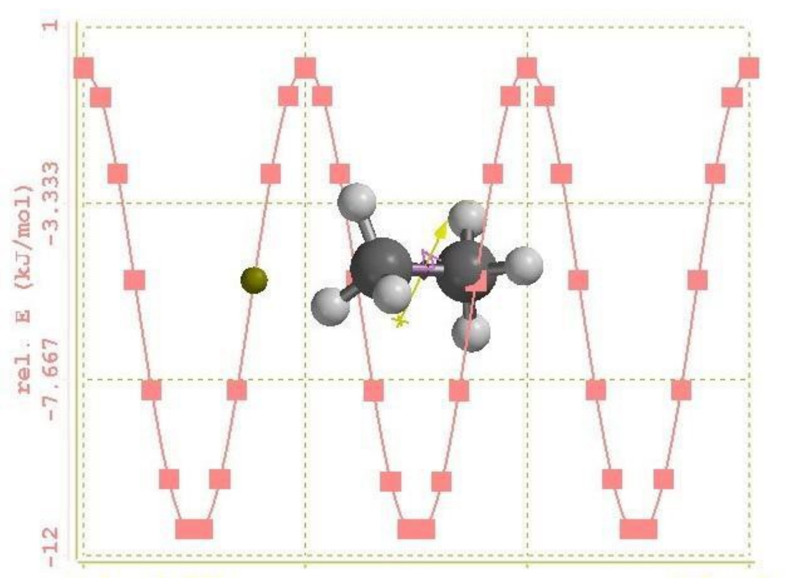

Figure 2. Rotation around a sigma(C–C) bond of ethane molecule and its impact on the energy of the molecule.

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Editorial updates

- Layout was processed into LUMAT-B template.
- The structure of the article was renewed through headings.
- Some typos corrected and text edited.
- Keywords added.
- Figure 1 was redrawn.
- Software section updated in order to match the current options available.
- References were processed into the APA style.