Computer animations in physical chemistry

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Introduction

The immense increase in computational power, variety of computer-based educational material and decreasing computer costs over the past few decades has increased the ease and importance of using computers in education. For example, most teachers use computers when preparing or presenting their courses. This can range from using publicly available programs to prepare notes and assessments to developing software to enhance the students' understanding of the course curriculum.

In addition, distance and internet-based learning requires advanced computational tools. The increased use of these types of learning methods presupposes development in computer hardware (such as video teaching and rapid information transfer) and software (*e.g.*, learning programs). These improvements are required to minimise the disadvantages associated with distance learning methods, such as the lack of face-to-face teacher-student contact, good assessment methods and laboratories for practical courses.

In most scientific and engineering subjects computers can be used to improve the presentation of course material and to increase students' understanding of important concepts. For example, power point is often used to present lectures or to prepare transparency overheads. This can be considered as a 'passive' use of computers since it is only the teachers, and not the students, that use the computers. An 'active' or 'hands-on' use of the computers requires that the students perform tasks on the computer. This can also range in complexity from simple implementations of existing programs to development of their own software.

The Physical Chemistry curriculum at the University College of Borås contains concepts that many students have difficulty in understanding. In addition, it is expected that students taking the course obtain a microscopic understanding of macroscopic properties, that is, how dynamics and reactivity at the atomic (and even quantum) level lead to chemical changes that are seen in everyday life and measured experimentally. A simple example is boiling water on a stove (*e.g.*, to cook rice). The physical chemist should have the understanding that water gets hotter (macroscopic property) since the water molecules increase their average speeds (and that they do this by adsorbing the heat from the stove). As the speed of the molecules increase the temperature increases towards 100°C. At this temperature the molecules move so fast (a physical chemist would express this in terms of their kinetic energy) that the bonds between the water molecules break, and the liquid phase water becomes a gas (*i.e.*, the water boils). Since this boiling yields more water molecules in the gas phase, there are more molecules that can collide with the lid of the saucepan. The increased collision frequency with the lid is commonly called an increase in pressure, and the lid lifts off the saucepan to release some of the water molecules into the environment (another macroscopic observable).

Traditional lectures and (wet) laboratories are not very well suited for conveying this microscopic understanding to the students. Instead, computer animations of the molecules can be used. Here students can view the motion of molecules on the computer and visualise how changes in the molecular properties leads to changes in certain macroscopic properties.

Also, it is preferable if the students can actively change the microscopic (macroscopic) property and view how it changes the macroscopic (microscopic) property.

In an effort to help students gain microscopic understanding of important physical and chemical concepts, we have introduced computer animation laboratories in the physical chemistry curriculum at the University College of Borås (a course for second year chemical engineers). These laboratories are not intended to substitute the existing traditional (wet) laboratories (in fact, these types of animations are sometimes referred to as computer experiments and can be thought of as a bridge between theory (lectures) and practice (wet laboratories). The implementation and evaluation of the computer laboratories are presented below.

Implementation of the computer animations.

The SimChemistry program for windows, which can be used for free for 30 days before registration and payment is required, was used for the computer laboratories. It can be downloaded from http://www.simchemistry.co.uk/. Although this program allows one to develop custom made animations, the preliminary laboratories discussed here used only the animations that accompany the program. These animations focus on the following six concepts:

1) Gases under pressure
2) Phases of matter
3) Mixtures of substances
4) Brownian motion
5) Enthalpy, activation energy and chemical equilibrium
6) Adsorption of gases at surfaces

A laboratory guide (Appendix A) was given to the students at the beginning of the course. It included information about SimChemistry, deadlines for laboratory reports (which coincided with lectures of these concepts) and simple questions that ensured that the students did the laboratories. Although the students had access to computers at the university college, most of them did these laboratories from home. Since the use of SimChemistry is very well explained in a tutorial that accompanies the program, hands-on supervision is not required. However, 10 minutes of the first course lecture was spent showing them the SimChemistry program.

Evaluation

Questionnaire

The computer laboratories were evaluated by asking the students to fill in a questionnaire (Appendix B). Each of the six laboratories was evaluated separately, and the students' attitudes to computer animations and to SimChemistry in general were investigated. The questions focussed on the ease with which SimChemistry can be implemented and used, as well as the relevance and interest in using computer simulations in physical chemistry (for each of the six concepts and in general). The questionnaire consisted of certain assertions that the students were required to rank on a scale of 1 to 4 whether they definitely disagreed (1), partially disagreed (2), partially agreed (3) or definitely agreed (4) with each assertion. The students were not required to partake in the evaluation as part of the course, but were encouraged to do so for the sake of the future course development.

Results

Completed questionnaires were received from thirteen of the nineteen students (some students did not answer all questions). Since this is a small number of replies, an in-depth analysis of the questionnaires has not been made. Instead, to gain an overview of the students' attitudes to the computer laboratories, the ranking of the assertions were grouped (number of students that ranked 1, number that ranked 2, *etc*). These are tabulated in Appendix C.

For the sake of brevity histograms were plotted for the first laboratory (Gases under pressure) and for the general questions regarding animations and SimChemistry. These histograms are shown in Appendices D and E, respectively.

The rankings are very similar for all six laboratories, and hence the histograms shown in Appendix D can be considered as typical for all laboratories. In summary, the students thought that:

i) All laboratories in SimChemistry were easy to run and were easy to understand.
ii) Atomic level understanding of physical chemistry concepts is important and interesting and that the computer laboratories deepen their understanding of these concepts.
iii) The laboratory questions were not difficult.
iv) Computer animations are not the only way to get atomic level understanding of physical chemistry concepts (the questionnaire did not allow them to identify other means to gain this understanding).

The histograms presented in Appendix E, for the general questions, show similar trends to those presented above. In addition, the students believe that:

i) Traditional (wet) laboratories and lectures are not sufficient to obtain atomic level understanding of physical chemistry concepts.
ii) Physical chemistry courses should not be based exclusively on wet laboratories, and that a combination of wet and computer laboratories is preferred.
iii) SimChemistry is easy to download and use, and although it has deepened the students understanding of the chemical concepts that were addressed in the laboratories, it should be used to address other, more difficult, concepts.

Conclusion and future plans

The students have a positive attitude towards computer simulations as a tool to deepen their microscopic understanding of physical chemistry concepts. They also feel that a microscopic understanding is important in their education. Although SimChemistry is easy to use and understand, they feel that the concepts that are treated are simple and they would like SimChemistry to be extended to treat difficult concepts.

These results indicate that, at least in the short term, implementation of computer animations in this course should:

i) Be based on SimChemistry
ii) Extend SimChemistry to include other concepts (this can be done by the teacher or the students).

In addition:

i) Due to the ‘simple’ concepts that SimChemistry treats, it can also be used at earlier stages in physical chemistry education (perhaps at the high school level).

ii) SimChemistry could also be used in other chemistry and chemical engineering courses.

Reference

1. *SimChemistry for Windows*. Copyright (c) 1996 - 2000 Charlie Wartnaby.

Appendix A

Computer laboratories:

There is no time set in the schedule for these laboratories. They must be done, either at home or in the computer rooms at the university (4th floor at IH or in the library), in your free time. Although you may discuss the laboratories with all of the class members, each laboratory group must hand in a report. The laboratory groups consist of two people and are the same groups as for the 'wet' laboratories.

The computer laboratories consist of five parts:

1. Run the computer program to understand an important concept in physical chemistry.
2. Answer the questions for each laboratory.
3. Suggest other questions that could be asked to improve your understanding of the physical chemistry.
4. Complete the evaluation forms regarding the use of animations in teaching.
5. Hand in the report (containing parts 2 and 3) before the deadline.

Deadlines

Lab 1.	12:00, Friday 5th September
Lab 2.	12:00, Monday 13th October

SimChemistry

The laboratories require the SimChemistry program which can be downloaded from www.wartnaby.demon.co.uk (get the zipped or unzipped version). There are some floppy diskettes available with this program. I suggest that you go through and understand the tour.scw file before proceeding with the other labs.

Laboratory 1

Expand (Gas under pressure)

Vad menas med adiabatisk och isotermisk expansion?
Vad händer med temperaturen och trycket när den ideala gasen expanderar i vakuum? Varför?
Vad händer med temperaturen och trycket när den reala gasen expanderar i vakuum? Varför (förklara med avseende på kinetiska och potential energi?
Vad händer med kolvarna när det externa trycket sänks till 0.1 N/m? Vad är det slutliga interna trycket?
Varför blir volymen i det isotermisk exemplet större än vad den blir i det adiabatisk exemplet?

Matter (Phases of matter)

Varför (på en molekyl nivå) rör sig kolven kring sitt jämviktsläge då T, p är konstanta?
Vad händer om man sänker T och håller p konstant?
Hur kan man se om molekylerna är i gasfas eller fast fas?
Varför rör sig molekylerna?
Hur undvika man defekter i fasta ämnen när de tillverkas?

Mixtures (Mixtures of substances)
Vad händer om man ökar bindningsenergin mellan de blå molekylerna? Varför?
Vad händer om man ökar temperaturen?
Vad händer om man minskar bindningsenergin mellan molekylerna i en kristall?
Vad ska man ändra för att få gas molekylerna att bilda en vätska?

Brownian (Brownian motion)
Varför rör sig rökpartiklarna slumpmässigt i luften?
Hur kan små luftmolekyler få en stor rökpartikel i rörelse?
Är rökpartiklarnas rörelse temperaturberoende? Varför?
Vad skulle hända med rökpartiklarna utan luftmolekylernas påverkan?
Varför går röken rakt upp (och inte neråt) om det inte blåser, utan är vindstilla?

Förslag till andra/bättre frågor….

Laboratory 2
Simple reactions (enthalpy, activation energy and equilibrium)
Hur påverkas bildningshastighet om man ökar temperaturen på hela systemet?
Vad händer om bildningsenergin för de gröna molekyler är lägre än för de blåa och röda?
Hur är bildningshastighet beroende av aktiveringsenergin?

Surfsci (adsorption of gases at surfaces)
Vad vill man uppnå då man ökar temperaturen av en metallytan i praktiken?
Kan man finna en sådan här reaktion spontan i naturen? Förklara.
När bör man avbryta ett sådant experiment vid höga temperaturer?
Gäller Langmuir isoterm vid höga eller låga temperaturer? Förklara.

Förslag till andra/bättre frågor….

Appendix B

Questionnaire for computer animations in physical chemistry

There are a number of statements below.
If **definitely disagree** with a statement give it ranking **1**,
if you **partially disagree** give it ranking **2**,
if you **partially agree** give it **3** and
if you **definitely agree** give it **4**

The questions are divided into seven sections. The first six are for each of the six computer laboratories (all sections have the same questions), and the seventh section is a general questionnaire regarding the use of SimChemistry and computer animations when learning Physical Chemistry.

Expand (Gas under pressure)

	RANK
It was difficult to run the computer program	
It was difficult to understand the animations	
This computer laboratory has deepened my understanding of the related chemical concept	
It is difficult to get atomic-level understanding of this concept without computer animations	
It is important to have atomic-level understanding of this concept in the syllabus	
It is interesting to have atomic-level understanding of this concept	
The laboratory questions were too difficult	

Matter (Phases of matter)

	RANK
It was difficult to run the computer program	
It was difficult to understand the animations	
This computer laboratory has deepened my understanding of the related chemical concept	
It is difficult to get atomic-level understanding of this concept without computer animations	
It is important to have atomic-level understanding of this concept in the syllabus	
It is interesting to have atomic-level understanding of this concept	
The laboratory questions were too difficult	

Mixtures (Mixtures of substances)

	RANK
It was difficult to run the computer program	
It was difficult to understand the animations	
This computer laboratory has deepened my understanding of the related chemical concept	
It is difficult to get atomic-level understanding of this concept without computer animations	
It is important to have atomic-level understanding of this concept in the syllabus	
It is interesting to have atomic-level understanding of this concept	
The laboratory questions were too difficult	

Brownian (Brownian motion)

	RANK
It was difficult to run the computer program	
It was difficult to understand the animations	
This computer laboratory has deepened my understanding of the related chemical concept	
It is difficult to get atomic-level understanding of this concept without computer animations	
It is important to have atomic-level understanding of this concept in the syllabus	
It is interesting to have atomic-level understanding of this concept	
The laboratory questions were too difficult	

Simple reactions (enthalpy, activation energy and equilibrium)

	RANK
It was difficult to run the computer program	
It was difficult to understand the animations	
This computer laboratory has deepened my understanding of the related chemical concept	
It is difficult to get atomic-level understanding of this concept without computer animations	
It is important to have atomic-level understanding of this concept in the syllabus	
It is interesting to have atomic-level understanding of this concept	
The laboratory questions were too difficult	

Surfsci (Surface adsorption of gases)

	RANK
It was difficult to run the computer program	
It was difficult to understand the animations	
This computer laboratory has deepened my understanding of the related chemical concept	
It is difficult to get atomic-level understanding of this concept without computer animations	
It is important to have atomic-level understanding of this concept in the syllabus	
It is interesting to have atomic-level understanding of this concept	
The laboratory questions were too difficult	

General questionnaire:

	RANK
Animations in chemical education	
Computer animations can increase my understanding of chemical concepts	
It is difficult to get this atomic-level understanding without computer animations	
It is important to have this atomic-level understanding of chemistry in the syllabus	
It is interesting to have this atomic-level understanding of chemistry	
Traditional (wet) labs are sufficient to give atomic-level understanding of chemistry	
Lectures are sufficient to give atomic-level understanding of chemistry	
Only traditional (wet) labs should be included in the physical chemistry syllabus	
A combination of wet and computer labs is best in physical chemistry education	
Animations of other chemical concepts (e.g., entropy and reaction orders) should also be included in the syllabus	
SimChem	
It was difficult to install/download SimChem on my computer	
Doing the SimChem introduction lab. made is easier to do the subsequent labs.	
SimChem treats chemical concepts that are easy to understand even without use of computer animations	
In general, SimChem has deepened my understanding of certain chemical concepts	

Additional comments and suggestions will be greatly appreciated and can be made on the back of the questionnaire

Appendix C

Analysis of the questionnaire for computer animations in physical chemistry

The first column in the analysis of each table gives the number of students that gave a ranking of 1 (definitely disagree), the second column the number of students that gave a ranking of 2 (partially disagree), the third column the number of students that gave a ranking of 3 (partially agree) and the fourth column the number of students that gave a ranking of 4 (definitely agree)

Expand (Gas under pressure) ANALYSIS

It was difficult to run the computer program	13			
It was difficult to understand the animations	10	2	1	
This computer laboratory has deepened my understanding of the related chemical concept			8	5
It is difficult to get atomic-level understanding of this concept without computer animations	1	2	8	2
It is important to have atomic-level understanding of this concept in the syllabus			4	7
It is interesting to have atomic-level understanding of this concept			1	12
The laboratory questions were too difficult	9	4		

Matter (Phases of matter) ANALYSIS

It was difficult to run the computer program	13			
It was difficult to understand the animations	11	1	1	
This computer laboratory has deepened my understanding of the related chemical concept	1	1	7	4
It is difficult to get atomic-level understanding of this concept without computer animations	1	4	7	1
It is important to have atomic-level understanding of this concept in the syllabus			4	7
It is interesting to have atomic-level understanding of this concept	1			12
The laboratory questions were too difficult	8	3	2	

Mixtures (Mixtures of substances) ANALYSIS

It was difficult to run the computer program	13			
It was difficult to understand the animations	10	2	1	
This computer laboratory has deepened my understanding of the related chemical concept	1	1	8	3
It is difficult to get atomic-level understanding of this concept without computer animations	1	4	7	1
It is important to have atomic-level understanding of this concept in the syllabus			5	6
It is interesting to have atomic-level understanding of this concept	1		1	11
The laboratory questions were too difficult	10	2	1	

Brownian (Brownian motion) ANALYSIS

It was difficult to run the computer program	13			
It was difficult to understand the animations	10	2	1	
This computer laboratory has deepened my understanding of the related chemical concept	1		10	2
It is difficult to get atomic-level understanding of this concept without computer animations	2	1	8	2
It is important to have atomic-level understanding of this concept in the syllabus			4	7
It is interesting to have atomic-level understanding of this concept	1			12
The laboratory questions were too difficult	8	3	2	

Simple reactions (enthalpy, activation energy and equilibrium) ANALYSIS

It was difficult to run the computer program	13			
It was difficult to understand the animations	11	2		
This computer laboratory has deepened my understanding of the related chemical concept		2	8	3
It is difficult to get atomic-level understanding of this concept without computer animations	1	4	5	3
It is important to have atomic-level understanding of this concept in the syllabus			3	8
It is interesting to have atomic-level understanding of this concept	1		1	11
The laboratory questions were too difficult	12		1	

Surfsci (Surface adsorption of gases) ANALYSIS

It was difficult to run the computer program	13			
It was difficult to understand the animations	12	1		
This computer laboratory has deepened my understanding of the related chemical concept		1	5	7
It is difficult to get atomic-level understanding of this concept without computer animations	1	2	7	3
It is important to have atomic-level understanding of this concept in the syllabus			3	8
It is interesting to have atomic-level understanding of this concept	1		1	11
The laboratory questions were too difficult	6	1	4	

General questionnaire:

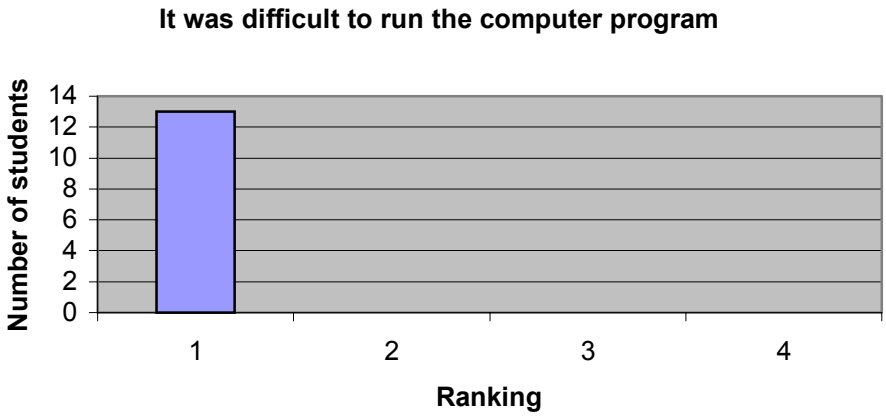
ANALYSIS

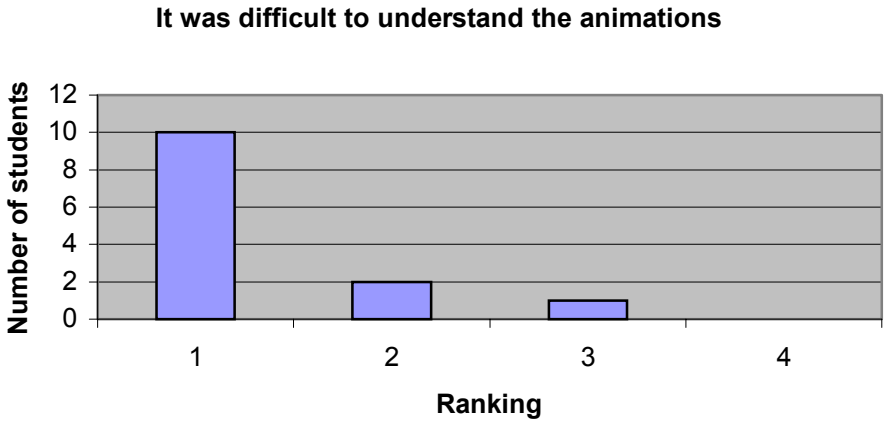
Animations in chemical education				
Computer animations can increase my understanding of chemical concepts			1	11
It is difficult to get this atomic-level understanding without computer animations		4	7	1
It is important to have this atomic-level understanding of chemistry in the syllabus		1	4	5
It is interesting to have this atomic-level understanding of chemistry			1	11
Traditional (wet) labs are sufficient to give atomic-level understanding of chemistry	1	10		1
Lectures are sufficient to give atomic-level understanding of chemistry	4	6	1	
Only traditional (wet) labs should be included in the physical chemistry syllabus	10	1		1
A combination of wet and computer labs is best in physical chemistry education				11
Animations of other chemical concepts (e.g., entropy and reaction orders) should also be included in the syllabus		1	2	8
SimChemistry				
It was difficult to install/download SimChem on my computer	10	1		
Doing the SimChem introduction lab. made is easier to do the subsequent labs.	1	2	5	1
SimChem treats chemical concepts that are easy to understand even without use of computer animations	2	7	1	
In general, SimChem has deepened my understanding of certain chemical concepts		1	5	6

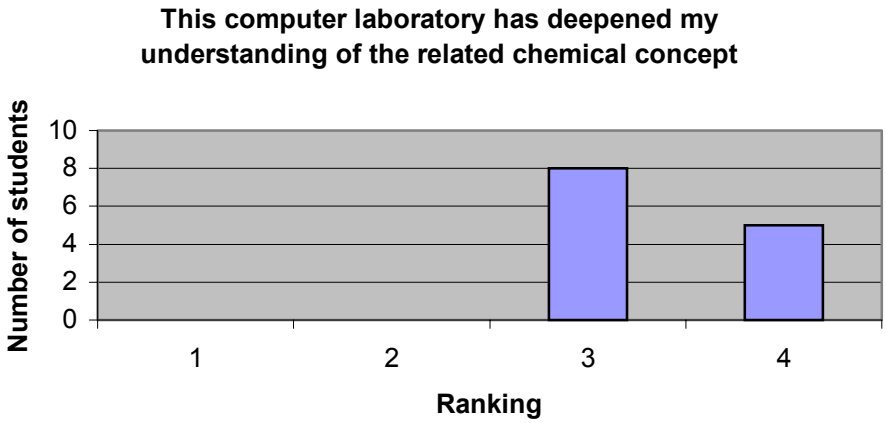
Additional comments:
Two students expressed great interest in having animations of other physical chemistry concepts.

Appendix D

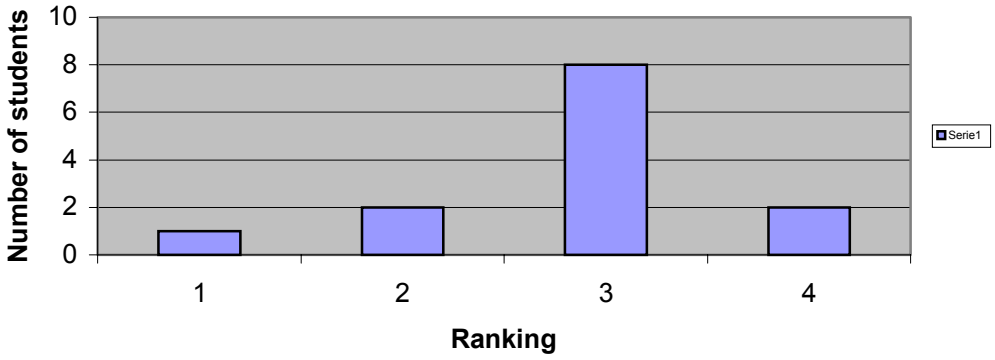
Histograms of the rankings for the 'Gases under pressure' computer laboratory



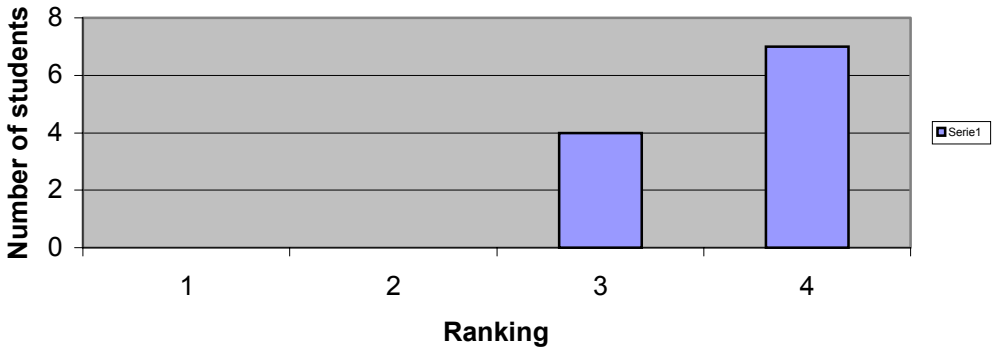




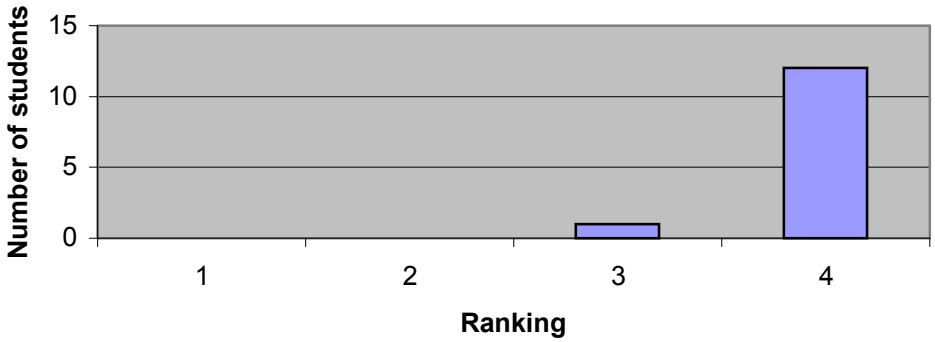
It is difficult to get atomic-level understanding of this concept without computer animations

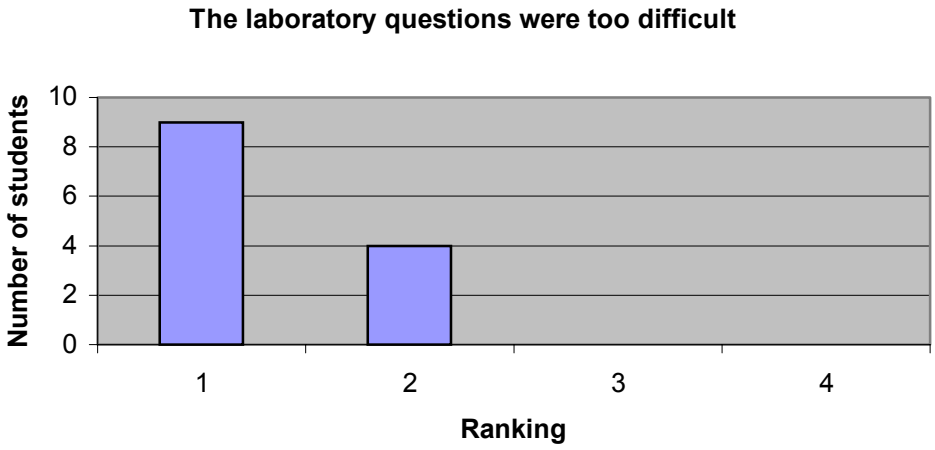


It is important to have atomic-level understanding of this concept in the syllabus



It is interesting to have atomic-level understanding of this concept




The laboratory questions were too difficult
Number of students
10
8
6
4
2
0
1
2
3
4
Ranking