# Emnerapport 2018 vår

# Emnekode: KJEM220

# Faglærers vurdering av gjennomføring

# Praktisk gjennomføring

The course introduced the students to the theory and practice of molecular modeling. The first part was dedicated to classical methods, such as molecular mechanics and dynamic simulations, while the second part focussed on quantum mechanical methods (Harthree-Fock, DFT, and an introduction to semiempirical methods). The course consisted in lectures (typically, two hours per week), guided discussions (one hour per week), theoretical exercises (two hours per week), and three practical, computational exercises. The practical component consisted in three sessions, each combining supervised, yet independent work at computer lab (from two to six hours), and homework mostly for analysis of the results and redaction of corresponding reports. These report were a compulsory component that, once delivered, commented and approved, granted access to the exam (four hours, written exam). Unapproved reports, could be edited according and re-submitted up to two times.

Traditionally, the computer exercises used to be the source of major practical challenges in organizing this class. However, the novel infrastructure made available by the HPC group of the IT-department solved most of the old issues.

# Strykprosent og frafall

More than half of the student registered to the course has never shown up nor manifested any intention to attend the course or give the exam. In fact, two of these admitted their registration was only meant to fill their study plan within the deadlines, without having any intention to follow this and many other coursers. The six active students attended regularly (more than 75% of the hours) and delivered the compulsory reports within the expected deadlines. Of these six, one has failed the exam.

In addition to the six active students mentioned above, and among the students whom have never attended any class, there were four more students registered to the exam. However, none of these was admitted to the exam due to lack of the compulsory requirements (i.e., approved reports of the computational exercises).

### Karakterfordeling

Grade	#	%
А	1	17%
В	3	50%
С	0	0%
D	0	0%
Е	1	17%
Failed	1	17%

### Studieinformasjon og dokumentasjon

All slides and exercises were uploaded into MittUiB, and the students evaluated this material positively (100% "good"). On the other hand, many students did not appreciate the textbook (i.e., A. Hinchliffe, "Molecular Modelling for Beginners", Wiley, 2008, second edition) or, as reported also to the lecturer, find it unclear and lacking examples and exercises (50% consider it "good", but 25% "bad", and 25% "very bad"). This was also pointed out in the questionnaire's section dedicated to anonymous suggestions.

# Tilgang til relevant litteratur

The book was not available in Studia until the 3<sup>rd</sup> week of the course. Apparently there has been some misunderstanding in the communications with Studia.

# Faglærers vurdering av rammevilkårene

# Lokaler og undervisningsutstyr

The classrooms and computer labs were usually in good conditions and suitable for the lectures.

Still, here is kind suggestion for improving the work environment. Rooms should be booked only via the centralized, online system and not by placing paper notes on the doors without even checking the pre-existing schedule. In three occasions, uncooperative personnel of the Chemistry department occupied the classroom that was officially booked for KJEM220. Luckily, thanks to the small number of active students, the lecturer managed to find an alternative solution, but not without loss of time.

# Andre forhold

Four weeks after the beginning of the course we discovered that the course schedule distributed to the students was wrong. In practice, some lectures had mistakenly been assigned to groups of students that did not include any of the actual students. Therefore, some of the students following the schedule on MittUiB have lost a few lectures in the initial part of the course, that is, until we figured out this problem. Importantly, the problem was not visible to the lectures in MittUiB, and it was identified only because some students systematically missed the lecture in a specific time slot.

# Faglærers kommentar til student-evalueringen(e)

# Metode – gjennomføring

Only 4 of the 6 active students answered the electronic questionnaire. Other four students were included in the panel, but did not respond nor attended any lecture.

### **Oppsummering av innspill**

A clear compulsion from the evaluation is the inadequacy of the textbook. There is significant room for improvement on this front, but, unfortunately, a good book covering the topics of this class with sufficient clarity and exercises is yet to be identified. In addition, the students underlined the very diverse backgrounds represented among them (Nanosciences, Biology, organic Chemistry, Physics). This heterogeneity represent a challenge that was not fully met since one out of four students considered his/hers own background knowledge inadequate. Moreover, 25% of the students describe the associated workload as higher than expected, which is also possibly due to inadequate background.

### Ev. underveistiltak

# Faglærers samlede vurdering, inkl. forslag til forbedringstiltak

- The quest for a proper textbook is clearly pivotal for the improvement of the course.

#### Kommentar til undersøkelsen:

Studentene får tilsendt evalueringsskjemaet 3 uker før eksamen, med svarfrist dagen før eksamen. I tillegg blir det sendt ut inntil to påminninger til de som ikke svarer etter første eller andre utsendelse/påminning.

Kun de studentene som har deltatt på mer enn 25% av forelesninger og kollokvier får oppfølgingsspørsmål om hva de synes om forelesninger/kollokvier. <u>Alle</u> som svarer at de har vært på færre enn 75% av forelesninger/kollokvier får imidlertid forklare hvorfor de ikke har deltatt på flere.

#### Oppfylte KJEM220 forventningene du hadde til kurset? Did this course meet your expectations?



#### Utdyp gjerne svaret ditt / Please elaborate:

#### Hvorfor har du valgt å delta på KJEM220? Why did you choose to attend this course?

- It will be relevant for future work
- Relevant for masterstudiet
- I had to
- Nødvendig

### Hvilke av de følgende kursene fra UiB har du fulgt tidligere? Please mark which of the following courses you have attended earlier?



# Har du annen relevant bakgrunn? / Please specify your relevant background

- I have a bachelor in chemistry engineering from what used to be HIB (høgskulen i bergen). I also had organometallic catalysis as special topic (10 points), expect that to be similar to kjem243.
- PHYS111, PHYS112, MAT112
- Kjemiingeniør

# Har du god nok bakgrunn til å ha fullt utbytte av undervisingen i KJEM220?

Did you feel your background knowledge was adequate to follow the content of this course?



Innenfor hvilke områder mener du at du manglet kunnskap på forhånd? Specify in which area you feel you would have benefitted from knowing more in advance:

### Hvor stor andel av forelesningene har du fulgt? How regulary have you attendend the lectures?



### Har du forberedt deg til forelesningene? Did you prepare yourself for the lectures by reading the curriculum ?



Klarhet i fremstillingen på forelsningene. 1 til 5, der 1 er meget uklar og 5 er meget klar.

How clear was the presentation of the different topics during the lectures? Rate on a scale from 1 to 5 (1=very unclear, 5=very clear)



Hvordan har læringsutbyttet av forelesningene vært? 1 til 5, der 1 er svært lavt læringsutbytte og 5 er svært høyt læringsutbytte. How good was your learning outcome from the lectures? 1 to 5, where 1 is very poor learning outcome and 5 is very high learning outcome.



Har forelesers spørsmål til studentene under forelesning og regneøvelser bidratt positivt til læringsprosessen?

The lectures and particularly the exercises were to a certain degree meant to be interactive with intermittent questions being posed by the lecturer. Do you think this approach helped you in your learning progress?



## Hvor stor andel av regneøvelsene (med penn og papir) har du fulgt? How large percentage of the colloquiums (pen and paper) have you attended?



Hvordan har læringsutbyttet av regneøvelsene (penn og papir) vært? 1 til 5, der 1 er svært lavt og 5 er svært høyt læringsutbytte. How was the learning outcome from the colloquiums (pen and paper)? Rate on a scale from 1 to 5 (1=very low learning outcome, 5=very high learning outcome)



Hvor stor andel av regneoppgavene har du gått gjennom på egenhånd? What proportion of the colloquium questions have you done on your own?



Kurset inneholder også tre obligatoriske øvelser basert på beregningskjemisk programvare. Hvordan har læringsutbyttet av disse øvlsene vært? 1 til 5, der 1 er svært lavt og 5 er svært høyt læringsutbytte.

The course also contains three compulsory exercises based on the use of computional chemistry software. How would you characterize the learning outcome of these exercises? Rate on a scale from 1 to 5 (1=very low learning outcome, 5=very high learning outcome)



### Fikk du hjelp på dataøvelsene når du trengte det? Did you get help to do computational excercises whwn you needed it?



### Ble dataøvelsene godt forklart av oppgaveteksten? Were the exercises well described in the text?



Hvor mange timer brukte du i snitt på hver av dataøvelsene (inkludert både tid på datalab og rapportskriving)? How many hours (including writing the report) did you use on average for each of the computational exercises?



Hva syns du om læreboken? 1 til 5 der 1 er svært bra og 5 er svært dårlig. /

What is your opinion of the textbook? Range on a scale from 1 to 5 (1=Very bad, 5=very good)



Hva synes du om presentasjonene som er lagt ut på MittUiB? What do you think about the presentations of the lectures presented on MittUiB?



Opplever du at det du har lært på KJEM220 vil være relevant for framtidige studier / forskningsaktiviteter? Do you think the knowledge you learned in this course will be relevant to your further studies / thesis / research activities?



10 studiepoeng skal i snitt tilsvare ca 13. t arbeid (organisert undervisning + egenaktivitet) per. uke. Hvor mange studiepoeng mener du emnet KJEM220 tilsvarer?

10 stp corresponds to a workload of approximately 13 h/week (lecturers and self study). How do you consider the amount of work involved in KJEM220?



Hvordan har kontakten med foreleser vært? 1 til 5, der 1 er svært dårlig kontakt og 5 er svært god kontakt.

How has the contact with the teaching staff been? Range on a scale from 1 to 5 (1=very poor contact, 5=very good contact)



#### Ris, ros, tips og utfyllende kommentarer til emnet som helhet? Feedback (positive and negative) and other more detailed comments regarding KJEM220?

- This class demands a lot of understanding and it can be hard to grasp sometimes even though the lectures are good. therefore it would be very helpful with book which thoroughly explain the concepts and provides examples. Even though the book has some assignments for some of the chapters (online which is very hard to find), it basically just provides us with a lot of equations, limited explanation and no examples.
- Øke studiepoengene for å forsvare arbeidsmengden