

Evaluation KJM5610/9610 - 2017

Also this year the course was mostly taken by exchange students, who are not at Master level, but they are at third-year bachelor. This creates a huge problem because their level, hardly possessing intuitive concepts of molecular orbitals and quantum numbers, with little or no knowledge of proper quantum mechanics, makes it impossible for them to follow what is supposedly an advanced course in electronic structure.

By proceeding with the lectures, it has been clear that the exchange students did not have the right background to follow the class. I had to reformulate major parts of the program to make the course of any usefulness for the students; still, only two of them took the exam.

As already pointed out in the last two years, I have difficulties finding KJM5610 a course that is appropriate for the chemistry students at UiO, even thinking to the reform going on. Its contents are too narrow, and thus it limits the number of students that are interested in it. Moreover, proper understanding requires very solid bases of quantum mechanics, quantum chemistry and computational skills, which will be anyway reached by a smaller niche of students.

Again, I am more than convinced that the KJM5630/5610 courses require a serious reshaping.

I propose to cancel them, and substitute them in the future Master program with the following two courses:

1 – Course in statistical mechanics and thermodynamics. This course may be offered at 4000- level, for those that want to anticipate it into the bachelor already. This should be a highly recommended course for the Master in physical chemistry, being statistical mechanics one of the two pillars, with quantum mechanics, on which all the fundamental understanding of matter in the condensed phase is based. Such a course, properly tailored in its contents for chemists (for example, including theory of liquids, elements of polymer science, protein folding, phase transitions etc) would be of high interest also for other disciplines like materials, catalysis or biochemistry.

2 – Course in multiscale molecular modeling

This course would follow logically from the former, but it would not strictly require it. It would cover some of the aspects today in KJM5630 related to modeling tools, and KJM5610 related to calculation of properties. The course should be very practical, with lots of hours in the computer lab, and a project-based evaluation. The projects should cover a vast gamma of methods, from quantum molecular structure and properties determination, to dynamical models in the condensed-phase, and properly named multiscale approaches.

This course would be also part of the portfolio of courses for the interdisciplinary Master in Computational Science, for which the Chemistry institute needs to offer a number of teaching hours.