

Theoretical and computational chemistry at the University of Oslo: our master portfolio

The theoretical chemistry group had a discussion concerning our master portfolio, with specific regards to the available courses given by our group, student requirements and demands, and available teaching resources.

Our findings and recommendations are as follows:

- While there are many ML-relevant aspects to most topics in theoretical and computational chemistry, there is a clear need for a course dedicated to the fundamentals of ML methods in a chemistry context. We recommend that KJM3610/4610 is given as soon as possible.
- We would like to introduce more code development and application in KJM5600.
- Many of our students would benefit from a theoretical course in many-body quantum theory, such as FYS-KJM4480, which was discontinued in 2017). We recommend the reintroduction of such a chemistry course open to physics students (for instance KJM-FYS4480).
- Practically all of Michele's students have been taking a special syllabus for statistical physics of polymers. They would likely benefit if this rather was given as a standard course on statistical physics of liquids and solutions.
- We lack some teaching resources, specifically:
 - David is hindered from teaching KJM3610 due to internal policy. This matter should be resolved before spring 2023.
 - Simen Kvaal is the ideal choice for giving the many-body theory course, only that he is currently employed as a researcher. It would be more appropriate to have him give this course as an associate professor.
 - We lack group teachers for KJM4310. This has been a problem for some years now.