Assessment KJM5630/9630 – 2018

The course was followed by a nine master students, and by one PhD student. The course was focused on different methodological methods aimed at conformational and phase space sampling, calculation of free energy differences, activation barriers and reaction rates.

The students were required to anchor intuitive computational experiment to basic theory involving statistical mechanics. All the mathematical formalism where explicitly presented and derived during the lectures. Lecture notes containing all passages were given to the students. The explanation of the fundamental algorithms for space sampling and molecular dynamics occurred by simple programming tasks for the students and by interactive analysis of trajectories for simple toy models, like harmonic oscillators. This year, the practical experiences were given a central role like in the past years. They were complemented by a set of discussions on research papers related to the topic of the course, and by a final group of special lectures on modeling tools for homogeneous catalysis by Dr. David Balcells. The course was well received by the students, who all passed the exam with high to very high marks.

This course has seen in the last few years a steady increase in the number of students. This is due to the participation of a growing number of students with a background different from a purely theoretical-computational one. This gives confidence on the fact, that in the new program, this course should be reformulated and expanded so to be of potential interest of the broadest possible audience.

Like written in the former assessments, I am convinced that this course would greatly profit from the contemporary institution of a full course in Statistical Mechanics for chemists, which would provide all the theoretical bases necessary for a clear understanding of the scientific bases behind the modeling techniques.