

COURSE INFORMATION

COMPUTATIONAL CHEMISTRY

Code number: 757509318(T1)

Degree in Chemistry

Academic Year: 2016-2017

Elective course. 4th year

Second semester: 3 credits

Tentative Schedule:

Classes start on the second half of the semester: Tu 11:00-13:30 and We 11:00-13:30. Classroom: Integrated Sciences Department seminar room. Experimental Sciences Building, fourth floor, red doors module.

TEACHING STAFF

Prof.: Francisco Pérez Bernal

Department: Integrated Sciences (Departamento de Ciencias Integradas)

Office: M1 P4-07 (Experimental Sciences building, red doors)

Phone: +34 959 219789

E-mail: francisco.perez@dfaie.uhu.es

Office hours:

First and second semester: Tu 16.00-18.00, We 12:00-14.00, Th 12:00-14:00

Students are invited to come to my office during office hours or at other times after a previous email appointment to discuss a homework problem or any aspect of the course.

SYLLABUS

1. DESCRIPTION

The present module aims to introduce students to some basic techniques for programming, scientific computing, and data analysis working with free software apps in a GNU/Linux operating system environment. This is a very practical subject where students will carry out basic calculations, preferably in problems of molecular or atomic structure, though depending of their background the development of applications in other fields is also possible.

2. PREREQUISITES

No prerequisites are defined apart from the fact that students should bring with them their laptops to class. The required software will be installed in their own computers. Students are expected to attend classes regularly and I highly encourage in-class participation. It can make a difference in the final grade.

3. OBJECTIVES/LEARNING OUTCOMES

- Acquire basic skills in GNU/Linux at the user and system administration level, with particular emphasis in a terminal approach instead of using GUI's.
- Develop user basic skills on several different applications of interests for chemists and scientists in general (e.g. LaTeX, Xmgrace, git, Inkscape etc.)
- Acquire basic programming skills using a modern language as Python in an Ipython + Emacs environment. Depending on the students background and

interests, other programming languages like Fortran90 or Perl could be addressed.

- Use of the Python library pandas for statistics and data treatment.
- Apply the aforementioned tools to atomic or molecular structure problems.

4. TEACHING METHODOLOGY

Classes will be mainly practical and students will follow the different activities with their laptops. Intensive use of Moodle is expected, where the major part of the documentation and links of interest can be found. Also students will find exercise assignments for the different items explained in class.

5. CONTENTS

- 1.- Basic user and admin GNU/Linux concepts. 2 hours
- 2.- UNIX. Use of the terminal. 5 hours
- 3.- Introduction to scientific programming in Python. 6 hours
- 4.- Scientific Applications in GNU/Linux. 3 hours
- 5.- Molecular and atomic structure and spectroscopy. Basic calculations. 8h

6. BIBLIOGRAPHY

Basic references

Wes McKinney. Python for Data Analysis: Data Wrangling with Pandas, NumPy, and Ipython. Ed. O'Reilly. 2013.

David B. Cook. Handbook of Computational Chemistry. Ed. Dover 2005.

Complementary references

R. L. Schwartz et. al. *Learning Perl*. Ed. O'Reilly. 2011.

Peter F. Bernath. *Spectra of Atoms and Molecules*. Ed. Oxford University Press. 2005.

Jeffrey I. Steinfeld. *Molecules and Radiation*. Ed. Dover. 2005.

A basic set of notes for FORTRAN 90 programming are also provided (Check [Basic_Fortran90_notes](#)). A large number of documents and links of interest are provided in Moodle.

7. ASSESSMENT/GRADING

GRADING BREAKDOWN

Coursework and exercise assignments 60%

Class participation 15%

Final assignment 20%

Exam 100% (Only for those students that had failed in the standard grading.)