Computational techniques in atomic and molecular structure, dinamics and spectroscopy

Academic Year: (2020 / 2021) **Review date: 22-04-2018**

Department assigned to the subject:

Coordinating teacher:

Type: Electives ECTS Credits : 3.0

Year : 2 Semester :

REQUIREMENTS (SUBJECTS THAT ARE ASSUMED TO BE KNOWN)

Introductory atomic and molecular physics.

OBJECTIVES

To introduce the basic computational tools to study atomic and molecular structure and dynamics with a practical point of view. Practical examples: Calculation of continuum wavefunctions; use of FFT to obtain momentum eigenfunctions; multireference calculation of potential energy surfaces for atoms and molecules; use of the R-matrix method; calculation of charge transfer (CXRS) cross sections of interest in fusion plasma diagnostic.

This course will provide the students the hand-skills computational techniques and programs to perform calculations and simulations on atomic and molecular structure and dynamics of interest in fusion plasmas

DESCRIPTION OF CONTENTS: PROGRAMME

1.- Atomic and molecular structure. Bound and continuum states. Variational, perturbational and model potential treatments. Molecular structure and symmetry. Ab-initio electronic structure of many-electron and of polyatomic molecules. Vibrational functions.
2.- Potential scattering and electron-atom collisions. The partial wave method. Transition probabilities. Different methods and tecniques in collisions of electrons with atoms and molecules. The R-matrix method. Excitation and ionization cross sections. Resonances.
3.- Atomic and molecular collisions. The semiclassical approximation. Close-coupling methods for ionization and charge transfer processes. Classical CTMC methods

LEARNING ACTIVITIES AND METHODOLOGY

* Teaching Methods:

Classroom lectures and classroom computational sessions. Homework assignments

* Course Material:

Lecture notes. Computational programs. Advanced references

ASSESSMENT SYSTEM

Evaluation shall take into account attendance and class participation, including practical classes, solution of questions, exercices and computational work to analyze an elementary system , including a theoretical introduction on one of the subjects proposed (50% of the final mark).

Written-closed book exam at the end of the semester (50% of the final mark).

% end-of-term-examination:	100
% of continuous assessment (assigments, laboratory, practicals…):	0

BASIC BIBLIOGRAPHY

- B.H. Bransden and M.H.C. McDowell Charge exchange and the theory of ion-atom collisions, Clarendon, Oxford, 1992
- F. Currell The physics of multiply and highly charged ions, Kluwer Acad. , 2003

- I. N. Levine QUANTUM CHEMISTRY, Allyn and Bacon Inc. Boston, 1983

- M. Karplus and R.N. Porter ATOMS & MOLECULES, Benjamin, Menlo Park, 1970

ADDITIONAL BIBLIOGRAPHY

- W H Press, S.A. Tukolsky, W. T. Vetterling, and B.P. Flannery Numerical Recipies, Cambridge University Press, 1992