Computational techniques in atomic and molecular structure, dinamics and spectroscopy

Academic Year: (2019 / 2020) **Review date: 22/04/2018 16:12:12**

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

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

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).

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