UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	**Name**
QF852	Molecular Modelling

Vector
OF:S-5 T:002 P:000 L:000 O:000 D:000 HS:002 SL:002 C:002 AV:N EX:S FM:75%

Pre requisite	None

Summary
Introduction to computer simulation methods, description of atomic and molecular models; chemical reactivity; biological systems; solids and material.

Program

A. Introduction to computational chemistry
Atomic and molecular models (*ab initio*, semi-empirical and DFT methods)
Electronic and molecular properties.
Applications.

B. Biological systems
Force fields.
Molecular Dynamics Simulations
Applications

C. Solids and materials
Computational chemistry in Nanoscience.
The Density Functional Theory revolution.
Applications.

Bibliography

[1] Métodos De Química Teórica E Modelagem Molecular
Autores: Nelson Morgon e Kaline Coutinho (Orgs)
Editora Livraria da Física, 2007

[2] Molecular Modelling – Principles and Applications
Autor: Andrew R. Leach
Ed. Prentice Hall, 2001

[3] Introduction to Computational Chemistry
Autor: Frank Jensen
Ed. Wiley, 1999

[4] Molecular Modeling Basics
Autor: Frank Jensen
Ed. CRC Press, 2010

Other references will be presented during the semester and will be specific for each topic.

Evaluation criteria
Evaluation criteria are defined by the Instructor on the bases of Section I – General Norms, Chapter V – Student Evaluation in the Subject, from the General Undergraduate Regiment. Attendance: 75 % (* Allowance for non-attendance will be considered according to Chapter VI, Section X, article 72 from the General Undergraduate Regiment).