Code: **QF852**

Name: **Modelagem Molecular**

Name in English: **Molecular Modelling**

Name in Spanish: **Modelización Molecular**

Subject type: **Weekly**

Approval Type: **Grade and Attendance**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering Period: **Semester / All periods**

Requires Final Exam: **Yes**

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
2	**-**	**-**	**-**	**-**	**-**	**2**	**15**	**2**

Occurrence on curriculum:

Pre requirement:

Summary: Introduction to computational simulation methods; description of atomic and molecular models; chemical reactivity; biological systems; solids and materials.

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.

Basic Bibliography

1) MORGON, N.; COUTINHO, K. **Métodos De Química Teórica E Modelagem Molecular** 1 Ed. São Paulo: Livraria da Física, 2007. 539 p.
2) LEACH, A.R. **Molecular Modelling – Principles and Applications** 2 Ed. Harlow: Prentice Hall, 2001. 744 p.
3) JENSEN, F. **Introduction to Computational Chemistry** 1 Ed. Chichester: Wiley, 1999. 429 p.

Supplementary Bibliography

1) JENSEN, F. **Molecular Modeling Basics** 1 Ed. Boca Raton: CRC Press, 2010. 166 p.
2) ROGERS, D.W. **Computational Chemistry using the PC** 3 Ed. Hoboken: John Wiley & Sons, 2003. 349 p.
3) FRENKEL, D.; SMIT, B. **Understanding Molecular Simulation**. 1 Ed. San Diego: Academic Press, 1996. 443 p.
4) LEWARS, E. **Computational Chemistry. Introduction to the Theory and Applications of Molecular and Quantum Mechanics.** 1 Ed. Norwell: Kluwer Academic Publishers, 2003. 471 p.
5) CRAMER, C.J. **Essentials of Computational Chemistry.**2 Ed. Chichester: Wiley, 2004. 596 p.