UNIVERSITY OF MAURITIUS
MODULE SPECIFICATION SHEET

1. GENERAL INFORMATION

Academic Year: 2011-2012
Semester(s): Annual

Title	Code	Duration (hrs)	N° of credits
Computational Chemistry	CHEM 2066	Lectures: 30	3
		Practicals: N/A	
		Seminars: N/A	
		Tutorials: 14	
		Others (Specify): Test: 1	
		Total: 45	

2. PRE-REQUISITE(S)/PRE-REQUIREMENT(S)

Knowledge of quantum chemistry

3. AIMS

To explain the following:
(1) Basics of computational chemistry
(2) Molecular Mechanics (MM) method
(3) Use of Chem Office
(4) *Ab initio* methods
(5) Hartree-Fock (HF) method
(6) Møller-Plesset perturbation theory (MP2) method
(7) Density Functional Theory (DFT) method
(8) Use of Gaussian 03W
(9) Use of GaussView
(10) Solvent effects
(11) Molecular dynamics

4. OUTLINE SYLLABUS

Computational Chemistry: its origin, development, future challenges and limitations, force fields and molecular mechanics, *ab initio* method, semi empirical theory, density functional theory, condensed phase calculations, molecular dynamics, applications.

5. LEARNING OUTCOMES

Having studied this module, the students should be able to:
(i) Understand applications of Computational Chemistry and its limitations
(ii) Understand and apply MM method to conformational isomers
(iii) Use Chemoffice software

(iv) Understand and apply HF method
(v) Understand and apply MP2 method
(vi) Understand and apply DFT method
(vii) Use Gaussian 03W software
(viii) Use Gauss view software
(ix) Apply *ab initio* methods to chemical problems
(x) Understand solvent effects
(xi) Apply molecular dynamics to specific problems

6. COORDINATORS:

	Programme Coordinator	**Module Coordinator**
Name	Assoc Prof S Jhaumeer-Laulloo	Assoc Prof P Ramasami
Department	Chemistry	Chemistry
Building	Tower block	Tower block
Room Number	3.8	3.8
Phone No.	4037505	4037506
E-mail address	sabina@ac.mu	p.ramasami@uom.ac.mu
Consultation Time	Office hours	Office hours

7. LECTURER(S)

Name	Assoc Prof P Ramasami
Department	Chemistry
Building	Tower block
Room Number	3.8
Phone No.	4037506
E-mail address	p.ramasami@uom.ac.mu
Contact Hours	45
Consultation Time	Office hours
Contact Address (For P/T)	

8. VENUE AND HOURS/WEEK

All lectures will normally be held in Room G2

Hours/week: 1.5 hours per week/ Friday 10 30 to 12 00

9. MODULE MAP

Wk(s)	Hr(s)	Theme(s)	Lecture Title(s)	Lecturer Initials	L, P, S, V, T, Test
1	1.5	Introduction	Computational chemistry, its applications and limitations	PR	L
2	1.5	MM method	Fundamentals of MM method	PR	L
3	1.5	MM method	Force field energy terms	PR	L
4	1.5	MM method	Advantages and limitations of MM method	PR	L
5	1.5	MM method	Applications of MM method to 1,2-disubstituted ethanes + revision of MM method	PR	L T
6	1.5	*Ab initio* methods	Introduction to Ab initio methods, advantages and limitations	PR	L
7	1.5	*Ab initio* methods	HF method, solution of Schrödinger equation (SE) equation	PR	L
8	1.5	*Ab initio* methods	HF method, solution of SE equation	PR	T
9	1.5	*Ab initio* methods	HF method, solution of SE equation + revision	PR	L T
10	1.5	*Ab initio* methods	MP2 method, extension of HF method	PR	L
11	1.5	*Ab initio* methods	MP2 method, advantages and limitations	PR	L
12	1.5	*Ab initio* methods	DFT method, introduction	PR	L
13	1.5	*Ab initio* methods	DFT method, advantages and limitations	PR	L
14	1.5	*Ab initio* methods	Revision of *ab initio* methods	PR	L
15	1.5	Gaussian 03W	Use of Gaussian 03W, input file, basis sets	PR	L
16	1.5	Gaussian 03W	Use of Gaussian 03W Optimisation, frequency, NMR calculations	PR	L
17	1.5	GaussView	Use of GaussView, input file	PR	L
18	1.5	GaussView	Use of GaussView, visualisations	PR	L
19	1.5	Applications	Atomisation energy, electron affinity, ionization energy	PR	L
20	1.5	Solvent effects	SCRF solvation models	PR	L

21	1.5	Solvent effects	SCRF solvation models	PR	L
22	1.5	Revision	Revision of topics covered weeks 15-21	PR	T
23	1.5	Molecular dynamics	Basics of molecular dynamics	PR	L
25	1.5	Molecular dynamics	Applications of molecular dynamics, limitations	PR	L
26	1.5	Revision	Discussion of assignments and examinations questions	PR	T
27	1.5	Revision	Discussion of assignments and examinations questions	PR	T
28	1.5	Class test	Class test	PR	T
29	1.5	Class test	Discussion of class test and examination questions	PR	T
30	1.5	Revision	Revision of topics covered	PR	T

Abbreviations: L: Lectures, P: Practicals, T: Tutorials, V: Visits, S: Seminars

10. RECOMMENDED BOOKS/JOURNALS/WEBSITES

(1) Physical chemistry, PW Atkins, 3rd edition or more recent
(2) Quantum Chemistry, I. N. Levine, 4th edition or more recent
(3) Exploring Chemistry with Electronic Structure Methods, JB Foresman and Æ Frisch, 2nd edition
(4) Introduction to Computational Chemistry, Frank Jensen, 1st Edition
(5) Websites (to inform)
(6) Journals (to inform)

11. ESSAY(S)/ASSIGNMENT(S)/PRACTICAL(S) (N/A)

12. ASSESSMENT

(i) **Written Examination**

Paper Structure	
Sections (if any): N/A	No. of questions to be answered: 2
Multiple Choice Questions: N/A	Compulsory Questions (if any): 1
Exams date: May 2012	Paper Duration: 2 hours
Weighting (%): 70	
Total Marks: 100	Pass Marks: 40

(ii) **Continuous Assessment**

	Weighting (%)
Assignment(s):	N/A
Practical(s):	N/A
Seminar(s):	N/A
Test(s):	30%
Total Marks:	30%