Computational Chemistry Applied to Electronic and Optical Organic Materials

CHEM 8873: Special Topic
Spring 2006

Lectures: Tuesdays and Thursdays 9:35 - 10:50
Classroom: Burger-Henry 357

Instructors:

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Goal of the course:

- To provide students, both experimentalists and theoreticians, with a **practical introduction** to the quantum-chemical methods that can be applied to determine the electronic, structural, and optical properties of organic materials.

- The emphasis will be on the description of: **electrically-active and optically-active organic materials**.

Goal of the course:

Upon completion of the course, the students will:

- have a working knowledge of the major quantum-chemical techniques;
- understand their main advantages and limitations
- be able to apply the quantum-chemical methods to simple cases; and
- better appreciate their relevance when reading the scientific literature.

Goal of the course:

The course will discuss, among others, the following organic materials:

- electrically conducting polymers;
- light-emitting molecules and polymers for displays and solid-state lighting;
- molecules and polymers for organic solar cells;
- chromophores for nonlinear optics with an emphasis on two-photon absorbers and molecules for electro-optics;
- hole-transport and electron-transport materials.

Structure of the course:

Each module of the course is divided into three sections:

- The first section introduces the **basic chemical** and **physical concepts** and discusses the current interest in the chosen materials;
  for instance, in the case of light-emitting organic materials:
  - what are the physical processes leading to luminescence?
  - what is a light-emitting diode?
  - how does it operate?
  - what are its applications in the market place?

Structure of the course:

Each module of the course is divided into three sections:

- The second section introduces the **quantum-chemical methods that are appropriate** to describe the relevant physical/chemical processes.

- The third section provides **hands-on experience** of the methods via selected examples.

Homeworks:

Will take the form of short reports describing briefly the results of calculations that will have been assigned.

There will be 4 or 5 during the semester.

Exams:

Mid-term:	February 28, 2006 (during class)
Final:	May 03, 2006 - 8:00-10:50 am
Take-home exam:	Due end of April

Points:

will be awarded in the following way:

- 100 points for the homeworks
- 100 points for the mid-term exam
- 100 points for final exam
- 100 points for take-home exam

Tentative Calendar

January

Sun	*Mon*	*Tue*	*Wed*	*Thu*	*Fri*	*Sat*
1	2	3	4	5	6	7
8	9	10 JLB – Module 1	11	12 JLB – Module 1	13	14
15	16	17 JLB – Module 2	18	19 DF – Module 3	20	21
22	23	24 DF – Module 3	25	26 JLB – Module 4	27	28
29	30	31 JLB – Module 4				

Module 1: Survey of the Main Quantum-Chemical Techniques
Module 2: Electronic Structure of Conjugated Polymers
Module 3: Hückel Theory
Module 4: Conducting Polymers

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Tentative Calendar

February

Sun	Mon	Tue	Wed	Thu	Fri	Sat
			1	2 JLB – Module 4	3	4
5	6	7 JLB – Module 4	8	9 JLB – Module 4,5	10	11
12	13	14 DF – Module 6	15	16 JLB – Module 7	17	18
19	20	21 JLB – Module 8	22	23 DF – Module 6	24	25
26	27	28 DF – MID-TERM				

Module 5: Electro-Magnetic Spectrum
Module 6: Using Electronic Structure Codes
Module 8: Light Emitting Plastics

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Tentative Calendar

March

Sun	Mon	Tue	Wed	Thu	Fri	Sat
			1	2 DF – Module 6	3	4
5	6	7 JLB – Module 9	8	9 JLB – Module 10	10	11
12	13	14 JLB – Module 10,11	15	16 KS – Module 12	17	18
19	20	21 **Spring Break**	22	23 **Spring Break**	24	25
26	27	28 KS – Module 12	29	30 KS – Module 12	31	

Module 9: Fluorescence-phosphorescence-Jablonski
Module 10: Transport
Module 11: Solar Cells
Module 12: TBA

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Tentative Calendar

April

Sun	Mon	Tue	Wed	Thu	Fri	Sat
						1
2	3	4 DF – Module 13	5	6 DF – Module 13	7	8
9	10	11 JLB – Module 14	12	13 JLB – Module 14	14	15
16	17	18 KS – Module 15	19	20 KS – Module 15	21	22
23	24	25 JLB – Review	26	27 DF – Review	28	29
30						

Module 13: Transport
Module 14: NLO
Module 15: TBA

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Tentative Calendar

May

Sun	*Mon*	*Tue*	*Wed*	*Thu*	*Fri*	*Sat*
	1	2	3 Final Exam	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30	31			

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