

INTRODUCTION TO ELECTRONIC STRUCTURE METHODS – CH-351

Mondays and Tuesdays 10h15 - 12h00

Date	Type	Description	
09.09. Mon	exercise	Exercise 1: Linear Algebra in Quantum Mechanics	Assistants
10.09. Tue	course	Intro & Repetition of basic QM & Linear Algebra	UR
16.09. Mon	—	Jeûne Fédéral	—
17.09. Tue	course	Basis Sets I	UR
23.09. Mon	course	Basis Sets II	UR
24.09. Tue	exercise	Exercise 2: Intro & HF calcs in Psi4	Assistants
30.09. Mon	course	Hartree-Fock I	UR
01.10. Tue	exercise	Exercise 3: Basis sets, De, geom opt.	Assistants
07.10. Mon	course	Hartree-Fock II	UR
08.10. Tue	exercise	Exercise 4: Hartree Fock procedure in detail	Assistants
14.10. Mon	exercise	Mock Exam with Old Written Exam	Assistants
15.10. Tue	exercise	Solutions of Mock Exam + Q&A Session	Assistants
21.10. Mon	—	Fall Break - No Classes	—
22.10. Tue	—	Fall Break - No Classes	—
28.10. Mon	exam	Written Exam I	Assistants
29.10. Tue	course	Configuration Interaction	UR
04.11. Mon	course BCH 1103	Many-Body Perturbation Theory	UR
05.11. Tue	exercise	Exercise 5: Post HF: MPn & CI	Assistants
11.11. Mon	course	Coupled Cluster Theory	UR
12.11. Tue	exercise	Exercise 6: DFT vs HF/MP2	Assistants
18.11. Mon	course	Multireference Methods (Andy)	UR/Andy

19.11. Tue	course	Density Functional Theory (DFT) I	UR
25.11. Mon	course	DFT II	UR
26.11. Tue	exercise	Exercise 7: Trouble Shooting, Pitfalls, traps	Assistants
02.12. Mon	course	DFT III (CP, QM/MM, Demos) & Summary	UR
03.12. Tue	exercise	Exercise 8: PES Scans	Assistants
09.12. Mon	exercise	Exercise 9: Transition States	Assistants
10.12. Tue	exercise	Q&A Session	Assistants
16.12. Mon	exam	Written Exam II	Assistants
17.12. Tue			