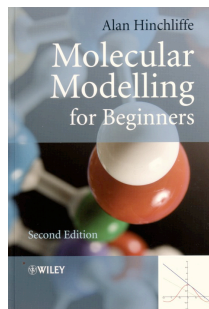


KJEM220 Fall 2014 – Reading List.

Primary textbook:
 A. Hinchliffe
Molecular Modelling for Beginners.
 Second Ed., (Wiley, 2008)



Including chapter	Excluding subchapter
1 Electric Charges and Their Properties.	9.2, 9.3, 12.1
2 The Forces Between Molecules.	10
3 Balls on Springs.	6
4 Molecular Mechanics.	1, 2
5 The Molecular Potential Energy Surface.	5, 6, 7, 8.2-8.4, 9, 11, 12
6 Molecular Mechanics Examples.	3, 4
8 Introduction to Statistical Thermodynamics.	3-5, 8
9 Monte Carlo Simulations	6, 7
10 Molecular Dynamics.	3.2, 6.1
11 Introduction to Quantum Modelling.	2, 4-6, 8-10
12 Quantum Gases.	1-5, 10
13 One-Electron Atoms.	1-3, 6, 10-12
14 The Orbital Model.	4, 8
15 Simple Molecules.	3-6, 7.1
16 The HF-LCAO Model.	3-7
18 Semi-empirical Models.	2-18
20 Density Functional Theory and the Kohn-Sham LCAO Equations	4

Also included in the curriculum are the computational exercises, paper & pen problems and topics for the discussion classes.