

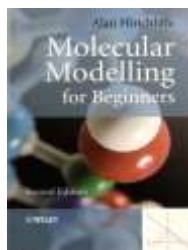
KJEM220 – Spring 2017 – Preliminary Reading List

Primary textbook:

A. Hinchliffe

Molecular Modelling for Beginners.

Second Ed., (Wiley, 2008)



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

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