课程名（Coursename）
Concepts in physical chemistry

课程代码（Coursenumber）
A6

课程对象（Audience）
Undergraduate

开课教师（Teacher）
Dr F. D. Pope and Dr J. A. Townsend

学期（Semester）
M 1–5

课程描述（Description）
This course is aimed at giving you a more detailed understanding of chemical bonding
than was possible in the Part IA course. This will require us to introduce some quantum mechanics, which we will do by taking an approach which is always firmly rooted in your chemical understanding and avoids excessive formality or mathematical detail. We will develop the key principles of quantum mechanics using simple model systems, which involve relatively easy mathematics, and then go on to see how these ideas can be applied in atoms and molecules. The course concludes by showing how molecular symmetry, in the form of group theory, can be used to great effect in drawing up MO diagrams of simple molecules.
Topics Revision of some basic mathematics. Functions and curve sketching (polynomials and trigonometric functions). The exponential function and logarithms. Differentiation: the chain rule; differentiation of a product. Integration. Introduction to complex numbers and the complex exponential.
Introducing quantum mechanics. What is quantum mechanics and why is it useful? Wavefunctions, operators and energy levels. Exemplifying these ideas for two simple systems.
Atomic orbitals. Review of AOs, their shapes and energies. Multi-electron atoms: the energies of singlets and triplets. Term symbols.
Molecular orbitals. The two orbital problem. Homo- and hetero-nuclear diatomics. Extended arrangements of orbitals (\_ systems) in rings and chains. Computational aspects.
Symmetry. How symmetry can help in constructing MOs. Introducing Group Theory. Using symmetry to construct MO diagrams.

课时信息（Totalhours）

教参信息（Textbookinfo）
Recommended books
1 Thermodynamics, Statistical Thermodynamics, & Kinetics (2nd Edition) by Thomas Engel and Philip Reid (Hardcover - Mar. 22, 2009)
ISBN-13: 978-0321615039
世界各地拥有馆藏的图书馆（OCLC）:66
2 Physical Chemistry for the Biological Sciences (Methods of Biochemical Analysis) by Gordon G. Hammes (Hardcover - Apr. 10, 2007)
ISBN-13: 978-0470122020
世界各地拥有馆藏的图书馆（OCLC）:322
3 Oxoacidity: reactions of oxo-compounds in ionic solvents (Comprehensive Chemical Kinetics) by Victor L. Cherginets (Hardcover - June 23, 2005)
ISBN-13: 978-0444517821
世界各地拥有馆藏的图书馆（OCLC）:120
4 Thermodynamics and Kinetics for the Biological Sciences by Gordon G. Hammes (Paperback - June 16, 2000)
ISBN-13: 978-0471374916
5 Statistical Thermodynamics: Fundamentals and Applications by Normand M. Laurendeau (Hardcover - Nov. 21, 2005)
ISBN-13: 978-0521846356
世界各地拥有馆藏的图书馆（OCLC）:172
6 Statistical Mechanics by Donald A. McQuarrie (Hardcover - May 2000)
ISBN-13: 978-1891389153
7 Thermodynamics, Statistical Thermodynamics, & Kinetics (2nd Edition) by Thomas Engel and Philip Reid (Hardcover - Mar. 22, 2009)
ISBN-13: 978-0321615039
世界各地拥有馆藏的图书馆（OCLC）:66
8 An Introduction to Thermodynamics and Statistical Mechanics by Keith S. Stowe (Hardcover - June 11, 2007)
ISBN-13: 978-0521865579
世界各地拥有馆藏的图书馆（OCLC）:170
9 Equilibrium and Non-Equilibrium Statistical Thermodynamics by Michel Le Bellac, Fabrice Mortessagne, and G. George Batrouni (Hardcover - May 3, 2004)
ISBN-13: 978-0521821438
世界各地拥有馆藏的图书馆（OCLC）:223
10 Thermodynamics and Statistical Mechanics (Classical Theoretical Physics) by Walter Greiner, Ludwig Neise, Horst Stöcker, and D. Rischke (Paperback - May 9, 1995)
ISBN-13: 978-0387942995
11 Introduction to Modern Statistical Mechanics by David Chandler (Paperback - Sept. 17, 1987)
ISBN-13: 978-0195042771