课程名（Coursename）  
Theoretical Techniques  
  
课程代码（Coursenumber）  
A4  
  
课程对象（Audience）  
Undergraduate  
  
开课教师（Teacher）  
Dr A. Alavi  
  
学期（Semester）  
M 1–5  
  
课程描述（Description））  
Rationalising molecular properties such as reactivity is a central goal of theoretical chemistry. Much qualitative insight can be obtained from molecular orbital theory. It is the aim of this course to introduce some theoretical techniques and ideas, such as perturbation theory, applied to MO calculations, which enable one to extract chemical insight. This course builds directly on the Quantum Mechanics, and Symmetry and Bonding courses you have met at Part IB.  
Topics Recap of Huckel theory; symmetry; linear and ring systems; population and bond-order analysis; alternant hydrocarbons; heteroconjugated systems; perturbation theory; reactivity theory; orbital correlation diagrams; molecular dissociation; molecular vibrations.  
  
课时信息（Totalhours）  
  
教参信息（Textbookinfo）  
Recommended books  
1 Theoretical and Computational Approaches to Interface Phenomena by J.T. Golab and H.L. Sellers (Hardcover - Feb. 28, 1995)  
ISBN-13: 978-0306448997  
2 Rarefied Gas Dynamics: Theoretical and Computational Techniques (Progress in Astronautics and Aeronautics) by E. P. Muntz, D. H. Campbell Weaver, and D. H. Campbell (Hardcover - July 1989)  
ISBN-13: 978-0930403553  
3 Hybrid Methods of Molecular Modeling (Progress in Theoretical Chemistry and Physics) by Andrei L. Tchougréeff (Hardcover - Aug. 6, 2008)  
ISBN-13: 978-1402081880  
世界各地拥有馆藏的图书馆（OCLC）:40  
4 Theoretical Advancement in Chromatography and Related Separation Techniques (NATO Science Series C: (closed)) by F. Dondi and Georges Guiochon (Hardcover - Oct. 31, 1992)  
ISBN-13: 978-0792319917  
5 Bioelectrochemistry: Fundamentals, Experimental Techniques and Applications by P. N. Bartlett (Hardcover - June 3, 2008)  
ISBN-13: 978-0470843642  
世界各地拥有馆藏的图书馆（OCLC）:113  
6 Multi-scale Quantum Models for Biocatalysis: Modern Techniques and Applications (Challenges and Advances in Computational Chemistry and Physics) by Darrin M. York and Tai-Sung Lee (Hardcover - June 30, 2009)  
ISBN-13: 978-1402099557  
世界各地拥有馆藏的图书馆（OCLC）:16  
7 Surface Analysis: The Principal Techniques by John C. Vickerman and Ian Gilmore (Paperback - May 18, 2009)  
ISBN-13: 978-0470017647  
世界各地拥有馆藏的图书馆（OCLC）:105  
8 Techniques in Inorganic Chemistry by John P. Fackler Jr. and Larry R. Falvello (Hardcover - July 16, 2010)  
ISBN-13: 978-1439815144  
世界各地拥有馆藏的图书馆（OCLC）:8  
9 Train Your Gaze: A Practical and Theoretical Introduction to Portrait Photography by Roswell Angier (Paperback - Nov. 15, 2006)  
ISBN-13: 978-2940373376  
世界各地拥有馆藏的图书馆（OCLC）:72  
10 Introduction to Thermal Analysis: Techniques and Applications (Hot Topics in Thermal Analysis and Calorimetry) by Michael E. Brown (Paperback - Dec. 31, 2001)  
ISBN-13: 978-1402004728  
世界各地拥有馆藏的图书馆（OCLC）:150  
11 Metallointercalators: Synthesis and Techniques to Probe Their Interactions with Biomolecules by Janice Aldrich-Wright (Hardcover - Nov. 29, 2010)  
ISBN-13: 978-3211094273  
世界各地拥有馆藏的图书馆（OCLC）:3  
12 The Basics of Theoretical and Computational Chemistry by Bernd Michael Rode, Thomas S. Hofer, and Michael D. Kugler (Hardcover - Mar. 26, 2007)  
ISBN-13: 978-3527317738  
世界各地拥有馆藏的图书馆（OCLC）:245