课程名（Coursename）
Electronic Structure

课程代码（Coursenumber）
C6

课程对象（Audience）
Undergraduate

开课教师（Teacher）
Prof. M. Sprik and Dr A. J. Cohen

学期（Semester）
L 6–8 & E 1–2

课程描述（Description））
The aim of this course is to provide an introduction to Electronic Structure theory, and in particular to go beyond the non-interacting, one-electron picture which has been implicitly assumed in the molecular orbital theory used in nearly all earlier courses. The inclusion of electron–electron repulsion is crucial for the quantitative prediction of molecular properties. Self-consistent field theory provides a way to include e-e repulsion, albeit at an approximate level maintaining a one-electron picture. Two varieties of SCF theory exist: wavefunction-based methods based on Hartree–Fock and density-functional methods. The former provides the traditional starting point to more systematic theories of electron correlation, and is the bedrock of quantum chemistry. The latter have proven a highly popular and efficient alternative to Hartree–Fock, but unlike Hartree–Fock, still account for electron correlation in an approximate way. Both topics will be covered.
Topics Basis functions, hydrogenic (Slater) orbitals, atomic orbitals, Gaussian functions, and contracted functions; the secular equations from which orbitals are determined; self-consistent field theory, and its numerical implementation; beyond Hartree–Fock, electron correlation; the energy functional, the importance of electron density, Hohenberg–Kohn theorems; The Kohn– Sham equations and orbitals; comparison with Hartree–Fock theory; the exchange correlation functional; electronic structure calculations as research tool.

课时信息（Totalhours）

教参信息（Textbookinfo）
1 Electronic Structure: Basic Theory and Practical Methods (v. 1) by Richard M. Martin (Paperback - Oct. 27, 2008)
ISBN-13: 978-0521534406
世界各地拥有馆藏的图书馆（OCLC）:37
2 Atomic and Electronic Structure of Solids by Efthimios Kaxiras (Paperback - Jan. 20, 2003)
ISBN-13: 978-0521523394
世界各地拥有馆藏的图书馆（OCLC）:265
3 Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond by Walter A. Harrison (Paperback - July 1, 1989)
ISBN-13: 978-0486660219
4 Molecular Electronic-structure Theory by Trygve Helgaker (Paperback - Aug. 30, 2010)
ISBN-13: 978-0470017609
世界各地拥有馆藏的图书馆（OCLC）:7
5 Electronic Structure Modeling: Connections Between Theory and Software by Carl Trindle and Donald Shillady (Hardcover - May 28, 2008)
ISBN-13: 978-0849384066
世界各地拥有馆藏的图书馆（OCLC）:150
6 Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory by Attila Szabo and Neil S. Ostlund (Paperback - July 2, 1996)
ISBN-13: 978-0486691862
7 Molecular Structure: Understanding Steric and Electronic Effects from Molecular Mechanics by Norman L. Allinger (Hardcover - Aug. 2, 2010)
ISBN-13: 978-0470195574
世界各地拥有馆藏的图书馆（OCLC）:27
8 Methods of Molecular Quantum Mechanics: An Introduction to Electronic Molecular Structure by Valerio Magnasco (Paperback - Jan. 12, 2010)
ISBN-13: 978-0470684412
世界各地拥有馆藏的图书馆（OCLC）:99
9 Computational Methods for Large Systems: Electronic Structure Approaches for Biotechnology and Nanotechnology by Jeffrey R. Reimers (Hardcover - Jan. 5, 2011)
ISBN-13: 978-0470487884
世界各地拥有馆藏的图书馆（OCLC）:4