课程名（Coursename）

Chemistry 242. Quantum Mechanics for Physical Chemistry

课程代码（Coursenumber）

2971

课程对象（Audience）

Primarily for Graduates

开课教师（Teacher）

Cesar Rodriguez-Rosario; Semion Saikin; Roel Sanchez-Carrera; Dmitrij Rappoport

学期（Semester）

Fall term

课程描述（Description））

Review of the fundamental principles of quantum mechanics: Hilbert spaces, operator algebra, Schrodinger, Heisenberg and interaction pictures. Approximate methods of solution of the Schrodinger equation: Perturbation, mean-field theories and the variational principle. Theory of chemical bonding: Effective Hamiltonian theories and molecular orbital theory. Symmetry and spectroscopy: Electronic, vibrational and NMR spectroscopy. Time-dependent quantum phenomena and its applications to chemical reaction dynamics: transition state theory and Marcus theory of electron transfer. Theory and applications of modern molecular electronic structure: Hartree Fock theory, density functional theory and Moller-Plesset Perturbation theory.

课时信息（Totalhours）

Tu., Th., 2:30–4. EXAM GROUP: 16, 17

教参信息（Textbookinfo）

1 Physical Chemistry: A Molecular Approach by Donald A. McQuarrie and John D. Simon (Hardcover - July 1, 1997)

ISBN-13: 978-0935702996

2 Quantum Mechanics in Chemistry (Physical Chemistry Textbook Series) by Melvin H. Hanna (Paperback - Feb. 1981)

ISBN-13: 978-0805337051

3 Introduction to Quantum Mechanics with Applications to Chemistry by Linus Pauling and E. Bright Wilson Jr. (Paperback - Mar. 1, 1985)

ISBN-13: 978-0486648712

4 Inorganic Chemistry by James House and James E. House (Paperback - Aug. 8, 2008)

ISBN-13: 978-0123567864

世界各地拥有馆藏的图书馆（OCLC）:207

5 Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics by Errol Lewars (Paperback - June 1, 2010)

ISBN-13: 978-9048138616

世界各地拥有馆藏的图书馆（OCLC）:2

6 Compendium of Quantum Physics: Concepts, Experiments, History and Philosophy by Daniel Greenberger, Klaus Hentschel, and Friedel Weinert (Hardcover - Sept. 9, 2009)

ISBN-13: 978-3540706229

世界各地拥有馆藏的图书馆（OCLC）:169

7 Quantum Mechanics in Chemistry (Topics in Physical Chemistry) by Jack Simons and Jeff Nichols (Hardcover - Jan. 30, 1997)

ISBN-13: 978-0195082005

8 Quantum Mechanics in Chemistry by George C. Schatz and Mark A. Ratner (Paperback - Jan. 28, 2002)

ISBN-13: 978-0486420035

世界各地拥有馆藏的图书馆（OCLC）:76

9 Molecular Quantum Mechanics by Peter Atkins and Ronald Friedman (Paperback - Feb. 17, 2005)

ISBN-13: 978-0199274987

世界各地拥有馆藏的图书馆（OCLC）:170

10 Beyond Measure: Modern Physics, Philosophy, and the Meaning of Quantum Theory by Jim Baggott and Peter Atkins (Paperback - Jan. 1, 2004)

ISBN-13: 978-0198525363

世界各地拥有馆藏的图书馆（OCLC）:470

11 Chemical Modeling: From Atoms to Liquids by Alan Hinchliffe (Hardcover - Nov. 1, 1999)

ISBN-13: 978-0471999034