课程代码（Coursenumber）  
Chemistry 7940 (794)  
  
课程对象（Audience）  
Primarily for Graduates  
  
开课教师（Teacher）  
Professor Ezra  
  
学期（Semester）  
Spring  
  
课程描述（Description）  
课程提纲（Syllabus）  
1. Approximation methods in QM: WKB theory  
• Motivation. Short-wavelength limit of Schr¨odinger equation.  
• WKB approximation. Conditions for validity.  
• Connection formulas.  
• Applications: 1D bound states. 1D barrier penetration.  
2. Density matrix  
• Pure vs mixed states. Ensemble interpretation.  
• Reduced density matrices.  
• Correlation & entanglement.  
• Equations of motion. Analogy with classical mechanics.  
• Relaxation and decoherence.  
3. Time-dependent phenomena  
• Evolution operator. Propagators and Green’s functions.  
• Three pictures: Schr¨odinger, Heisenberg, interaction.  
• 2-level system. Rotating wave approximation. Bloch equations.  
• Time-dependent perturbation theory. Harmonic perturbations. Resonant phenomena. Transitions  
to a continuum. Fermi’s Golden rule.  
• Sudden approximation.  
• Adiabatic approximation. A geometric phase.  
• Perturbation theory for the density operator. Linear response.  
4. Path integral formulation of quantum mechanics  
• Derivation of the sum-over-paths expression for the propagator.  
• Semiclassical limit of the path integral.  
5. Molecule-field interactions  
• Maxwell’s equations, scalar and vector potentials, gauge transformations, free field, and all  
that.  
• Hamiltonian for charged particle in field.  
• Perturbation in dipole approximation.  
• A and B coefficients. Selection rules. Sum rules.  
• Electric quadrupole and magnetic dipole transitions.  
• High-order perturbation theory and multiphoton processes.  
1 of 2  
• Nonlinear spectroscopy.  
• Electric properties of molecules. Polarizability.  
• Magnetic properties of molecules. Magnetic susceptibility. Diamagnetism & paramagnetism.  
• Quantizing the EM field. Photons. Spontaneous emission revisited.  
6. Quantum mechanics of the continuum: Scattering theory  
• Particle flux and scattering cross sections.  
• Green’s functions and the scattering problem.  
• Born approximation.  
• Partial wave analysis of wavefunction for central scattering potential.  
• Phase shifts and differential cross section.  
7. Molecular electronic structure  
• We are not addressing this topic, as the subject is being treated in detail by Professor Chan  
in Chem 7980, Bonding in Molecules.  
If we have time:  
8. Molecular vibrations  
• Born-Oppenheimer approximation.  
• Rotation-vibration separability.  
• Normal modes.  
• Vibration-rotation transitions. Selection rules. Polarization.  
  
课时信息（Totalhours）  
16696 LEC 001 TR  
03:00PM - 04:30PM  
CLK 609  
Hines,M (mah11  
  
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）:77  
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