课程名（Coursename）  
Computational Quantum Mechanics of Molecular and Extended Systems  
  
课程代码（Coursenumber）  
 5.675J  
  
课程对象（Audience）  
Graduate  
  
选课前提（prerequisite）  
Permission of instructor  
  
单元（units）  
3-0-6  
  
添加至时间表 （add to schedule）  
  
开课教师（Teacher）  
B. L. Trout  
  
学期（Semester）  
fall term  
  
课程描述（Description）  
The theoretical frameworks of Hartree-Fock theory and density functional theory are presented as approximate methods to solve the many-electron problem. A variety of ways to incorporate electron correlation are discussed. The application of these techniques to calculate the reactivity and spectroscopic properties of chemical systems, in addition to the thermodynamics and kinetics of chemical processes, is emphasized. Focus on cutting edge methods to sample complex hypersurfaces, for reactions in liquids, catalysts and biological systems. Students run computations both on Athena and on multi-processor supercomputers.  
  
备注（notes）  
H-level Grad Credit  
Same subject as 10.675J  
  
教参信息（Textbookinfo）  
None