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| |  | | --- | | 课程代码（Coursenumber） CHEM 276  课程对象（Audience） Primarily for Graduates  开课教师（Teacher） Andersen, H.  学期（Semester） Terms: Aut  课程描述（Description）） The statistical mechanical basis for computer simulations of atomic and molecular liquids. Principles of the Monte Carlo method, Metropolis algorithm, and application to lattice models and continuum fluids. Principles of molecular dynamics calculations, methods for sampling equilibrium ensembles, algorithms for dynamics. Periodic boundary conditions, methods for dealing with long-ranged forces, construction of potential energy functions, estimation of statistical error in results of simulations. Prerequisite: 275. it might be repeatable for credit.  课时信息（Totalhours） Units: 3  教参信息（Textbookinfo） The Chemical Dynamics and Kinetics of Small Radicals (Advanced Series in Physical Chemistry, Vol 6) by Kopin Liu and Albert Wagner (Hardcover - Sept. 1995) 1 Advanced Organic Chemistry: Part A: Structure and Mechanisms (Advanced Organic Chemistry / Part A: Structure and Mechanisms) by Francis A. Carey and Richard J. Sundberg (Paperback - June 13, 2007) ISBN-13: 978-0387683461 世界各地拥有馆藏的图书馆（OCLC）:228 2 Modern Trends In Chemical Reaction Dynamics: Experiment And Theory (Advanced Series in Physical Chemistry) (Pt. 2) by Xueming Yang and Kopin Liu (Hardcover - Nov. 28, 2004) ISBN-13: 978-9812389237 世界各地拥有馆藏的图书馆（OCLC）:121 3 Overview's of Recent Research on Energetic Materials (Advanced Series in Physical Chemistry) by Robert W. Shaw; Thomas B Brill; Donald L Thompson (Hardcover - Aug. 30, 2005) ISBN-13: 978-9812561718 世界各地拥有馆藏的图书馆（OCLC）:100 4 Conical Intersections: Electronic Structure, Dynamics & Spectroscopy (Advanced Series in Physical Chemistry) by Wolfgang Domcke, David R. Yarkony, and Horst Koppel (Hardcover - Oct. 2004) ISBN-13: 978-9812386724 世界各地拥有馆藏的图书馆（OCLC）:118 5 Carbon Nanotubes: Advanced Topics in the Synthesis, Structure, Properties and Applications (Topics in Applied Physics) by Ado Jorio, Gene Dresselhaus, and Mildred S. Dresselhaus (Hardcover - Mar. 11, 2008) ISBN-13: 978-3540728641 世界各地拥有馆藏的图书馆（OCLC）:114 6 Sol-Gel Materials: Chemistry and Applications (Advanced Chemistry Texts) by John D. Wright and Nico A.J.M. Sommerdijk (Hardcover - Dec. 21, 2000) ISBN-13: 978-9056993269 7 Advanced Batteries: Materials Science Aspects by Robert A. Huggins (Hardcover - Dec. 10, 2008) ISBN-13: 978-0387764238 世界各地拥有馆藏的图书馆（OCLC）:117 8 Photo-Excited Processes, Diagnostics and Applications: Fundamentals and Advanced Topics by A. Peled (Hardcover - Dec. 31, 2003) ISBN-13: 978-1402075278 世界各地拥有馆藏的图书馆（OCLC）:75 9 Transition Metal Carbonyl Cluster Chemistry (Advanced Chemistry Texts, Volume 2) (v. 2) by Paul J. Dyson and J. Scott McIndoe (Hardcover - Nov. 17, 2000) ISBN-13: 978-9056992897  10 Chemical Thermodynamics: Advanced Applications by J. Bevan Ott and Juliana Boerio-Goates (Hardcover - July 11, 2000) ISBN-13: 978-0125309851 | |