课程名（Coursename）  
Energy Landscapes and Intermolecular Forces  
  
课程代码（Coursenumber）  
M4  
  
课程对象（Audience）  
Graduates  
  
开课教师（Teacher）  
Prof. D. J. Wales, Dr D. Chakrabarti, and Dr J. Green  
  
学期（Semester）  
  
课程描述（Description）  
In the first part of the course we consider the relation between the observed molecular dynamics and thermodynamics and the underlying potential energy surface. This approach represents the natural extension of two state isomerization to complex systems with vast numbers of local minima. In small systems, such as HF dimer and water trimer, it is possible to characterise all the important minima and the transition states that link them, and deduce tunnelling splitting patterns. For large systems, the objective is to understand why some molecules are able to locate their global minima easily, whilst others are readily trapped as glasses.  
Although chemistry is concerned largely with reactions in which bonds are broken and re-formed, the forces between unreacting molecules and fragments of molecules are often of great importance, and are the subject of the second part of this course. It has been understood for many years that the attractive forces between molecules are responsible for the very existence of condensed phases, but only very recently has it become possible to build sufficiently detailed models of these forces to explain the complex behaviour of real liquids. The structures of complex biological molecules such as proteins and nucleic acids are controlled by “intermolecular” interactions between different parts of the molecule.  
Energy Landscapes  
Topics Introduction The study of potential energy surfaces, or“energy landscapes”, is of central importance in understanding the structure, dynamics and thermodynamics of any system of chemical interest. In particular, the potential energy surface holds the key to understanding how complex molecules such as proteins can locate their native state easily, while glass formers fail to crystallize.  
Stationary Points and Pathways The Born-Oppenheimer approximation. Symmetry properties of stationary points, pathways and mechanisms. Tunnelling Experimental manifestations. e.g. (HF)2. Searching the Landscape Geometry optimization and characterization of reaction mechanisms. Static and Dynamic Properties Thermodynamics from the superposition approach. Master equation dynamics. Global optimization. Describing Multi-Dimensional Surfaces How many stationary points? How are they connected? Visualization through disconnectivity graphs. Examples, including the annealing of C60 and the folding of a model protein.  
Intermolecular Forces  
Topics Overview Summary of the main contributions to the interaction energy and their characteristics. Magnitude of intermolecular forces. Why these weak forces are so important. Perturbation theory Intermolecular perturbation theory. The physical components of the interaction energy: electrostatic, induction and dispersion. Exchange effects. Asymptotic expansions The asymptotic form of the interaction operator and how it can be used to obtain asymptotic forms for the interaction energy components.  
Molecular properties The multipole moments and frequency-dependent polarizabilities determine the asymptotic form of the interaction energy. These will be discussed in some detail together with ways of distributing them over multiple sites. Current developments Density functional theory. Symmetry-adapted perturbation theories.  
  
课时信息（Totalhours）  
  
教参信息（Textbookinfo）  
1 5 Steps to a 5 AP Chemistry, 2010-2011 Edition (5 Steps to a 5 on the Advanced Placement Examinations Series) - Paperback (Nov. 11, 2009) by John Moore and Richard H. Langley  
ISBN-13: 978-0071624770  
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2 Chemistry and Physics for Nurse Anesthesia: A Student Centered Approach - Paperback (June 15, 2009) by Dr. David Shubert PhD and Dr. John Leyba PhD  
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3 West-E/Praxis II Chemistry 0245: Teacher Certification Exam (Xam West-E/Praxis II) - Paperback (May 1, 2008) by Sharon Wynne  
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