

NATIONAL TSING HUA UNIVERSITY
DEPARTMENT OF POWER MECHANICAL ENGINEERING
2011 Spring Semester

Course No.: PME 5153 00
Course Title: **Molecular Dynamics (分子動力學)**
Credits: 3
Hours/Week: M4W3W4
Classroom: 工一 209
Teacher: Prof. Che-Wun Hong (洪哲文 教授)

Contents:

- (1) Introduction to Molecular Dynamics
- (2) Hard Sphere Models
- (3) Computational Methods
- (4) Soft Sphere Models
- (5) Static Properties
- (6) Dynamic Properties
- (7) Number Density, Pressure and Microcanonical Ensemble
- (8) Potential Models
- (9) Monte Carlo Methods
- (10) Molecular Quantum Mechanics

Textbooks:

Course notes will be provided in pdf before each lecture

References:

- Basic: [1] "Molecular Dynamics Simulation Elementary Methods", J. M. Haile, John Wiley & Sons, Inc., 1997
- Advanced: [2] "Molecular Modelling Principles and Applications", A. R. Leach, 2nd Edition, Prentice Hall, 2001
- [3] "Molecular Quantum Mechanics", P. Atkins, R. Friedman, Oxford Univ. Press, 2005

Grades: Midterm Exam. (40%)
Midterm Report (30%) Final Report (30%)