A Winter Short Course on Statistical Mechanics for Molecular Simulations (2015)

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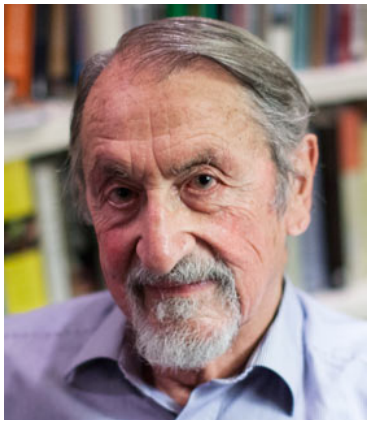
@ 121, Chemistry Building

2013 年諾貝爾化學獎

- 2013 Nobel Chemistry Prize jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.
- 複雜系統多層級計算方法的建立
- **將化學實驗帶入電腦**時空



Martin Karplus

Michael Levitt

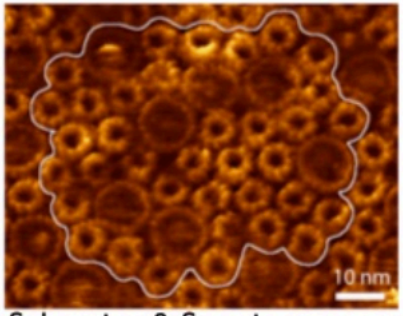
Arieh Warshel

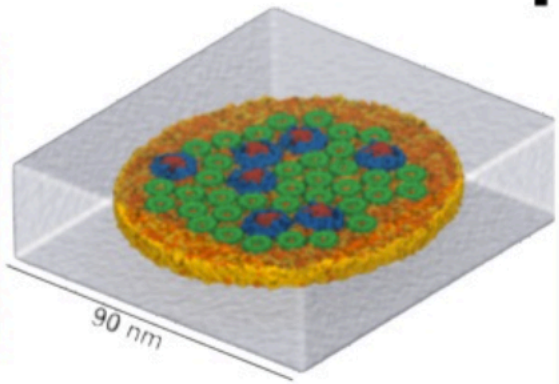
Pictures from nobelprize.org

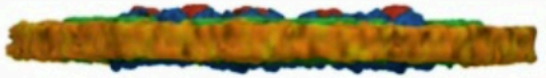
Slide from Prof. Jhih-Wei Chu

Whole chromatophore membrane

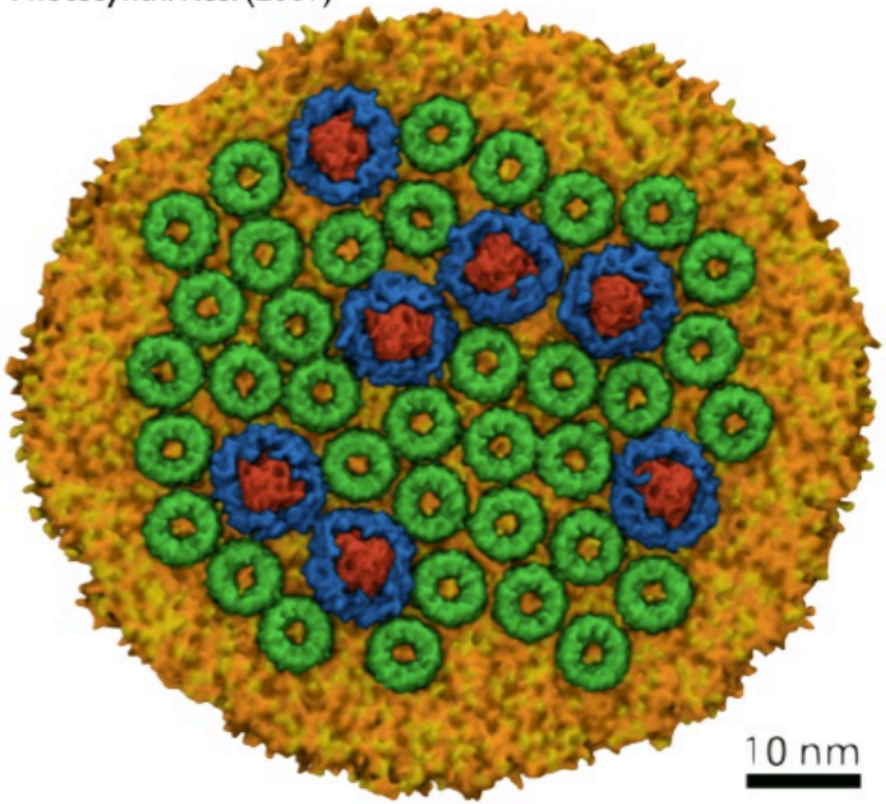
Rhodospirillum Photometricum







Scheuring & Sturgis
Photosynth. Res. (2009)



20 Million atoms
Simulated with NAMD 2.9
on Blue Waters
40 ns so far

Chandler, Strümpfer, Sener & Schulten. (2012) In preparation.

Course Information

- Webpage: http://quantum.ch.ntu.edu.tw/ycclab/teaching/winter-short-course-2015/

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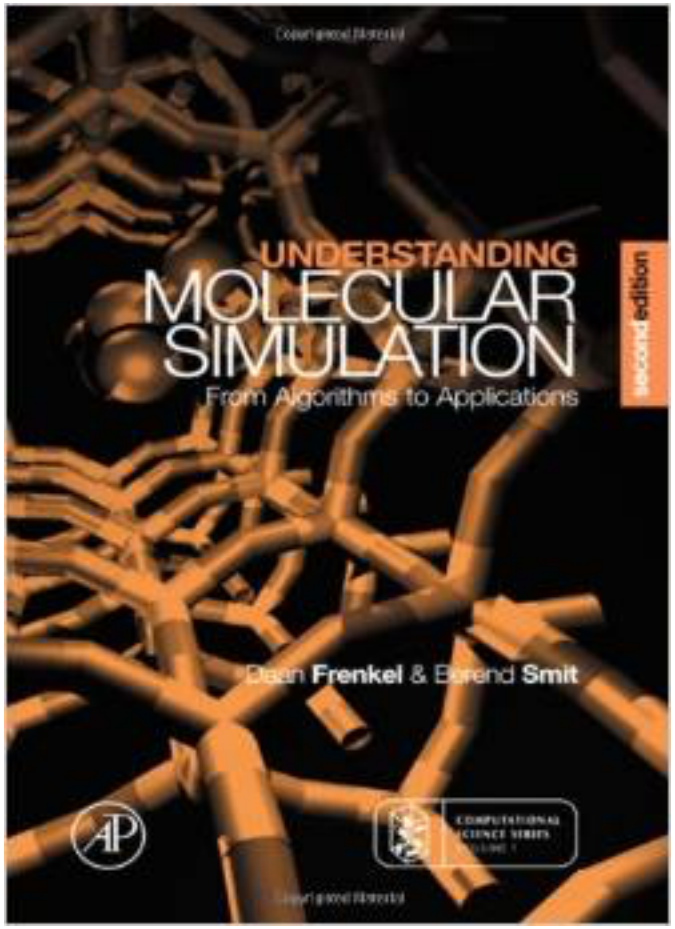
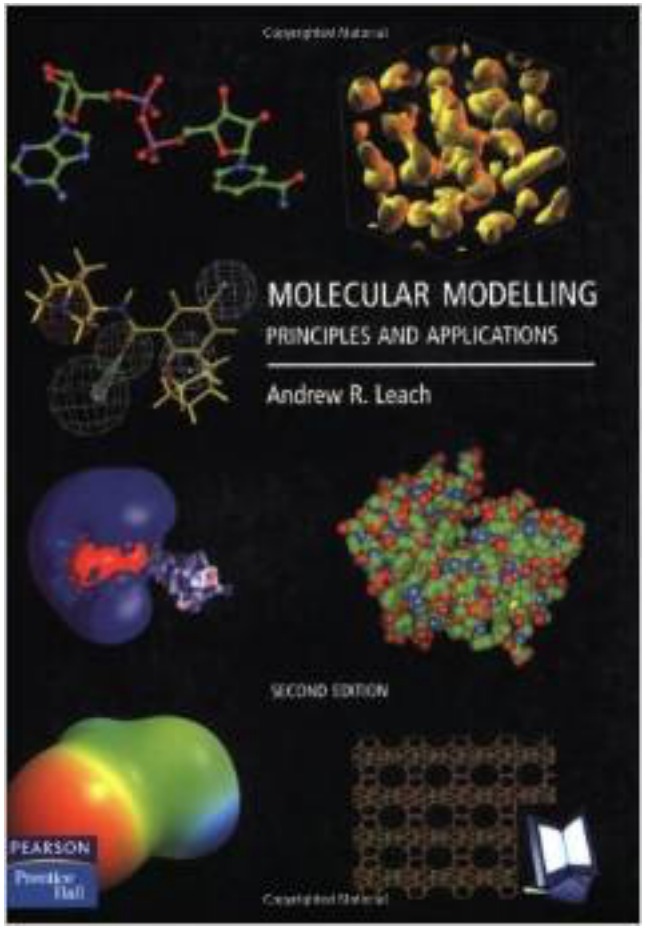
Tentative Schedule

- Statistical Mechanics (1/22, 1:30PM)
- Molecular modeling and interactions (2/2, 1:30PM)
- Monte Carlo simulations (2/4, 1:30PM)
- Molecular dynamics simulations (2/6, 1:30PM)
- Free energy calculations (2/9, 1:30PM)
- Non-equilibrium systems – I (2/11, 1:30PM)
- Non-equilibrium systems – II (2/13, 1:30PM)
- Location: Room 121

References


UNDERSTANDING
MOLECULAR
SIMULATION
From Algorithms to Applications
second edition
Daan Frenkel & Berend Smit
AP


MOLECULAR MODELLING
PRINCIPLES AND APPLICATIONS
Andrew R. Leach
SECOND EDITION
PEARSON
Prentice Hall

Scripting Lecture Notes

Statistical mechanics for molecular simulations. (2015) ①

Lecture 1 1/22/2015.

Fundamentals of statistical mechanics.

* ensemble theory
* two postulates of Stat. mech.
* microcanonical ensemble
* canonical ensemble.
* thermodynamic limit.

first lecture!
1. list of attendees.
2. textbook / references
3. open/informal environment.
4. background check.
5. web resources & course details.

* Course description / details.

http://quantum.ch.nsu.edu.tw/yclab/winter-shore-course-2015

Molecular simulations have become invaluable tools for researchers in chemistry, physics, biology, & material science. This shore course aims to provide the basic theoretical background that should better prepare you to understand / interpret the results of molecular simulations.

② Of course, we can only present a very brief introduction to the very fundamentals here. Two things I want to discuss in particular ⇒ entropy & Boltzman distribution.

⇒ but, yes, I want to teach you statistical thermodynamics in a week !!

* ensemble theory.

Modern stat. mech. is presented using ensemble theory as its foundation.

Macroscopic systems are too complicated, we can not track all microscopic / molecular motions of all particles in a bulk system ⇒ we can only consider "averaged" quantities.

key ⇒ a macroscopic (thermodynamic) state actually is consist of many-many "microstates".