

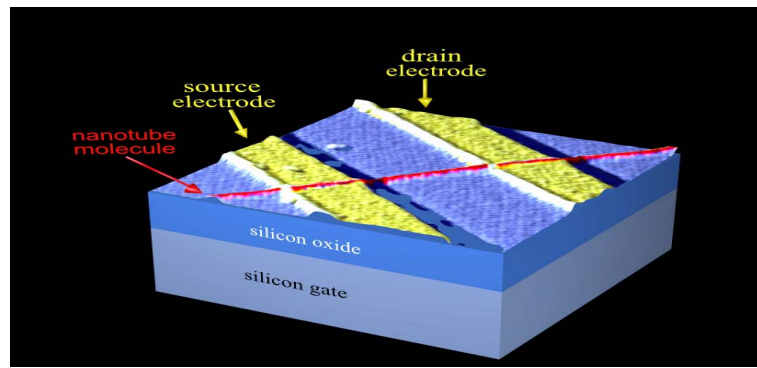
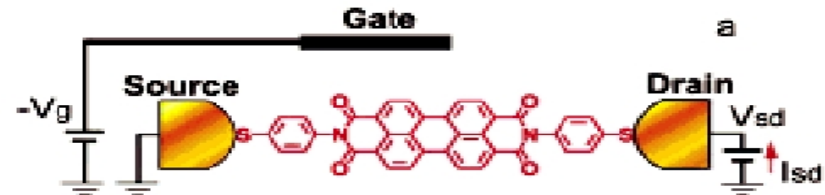
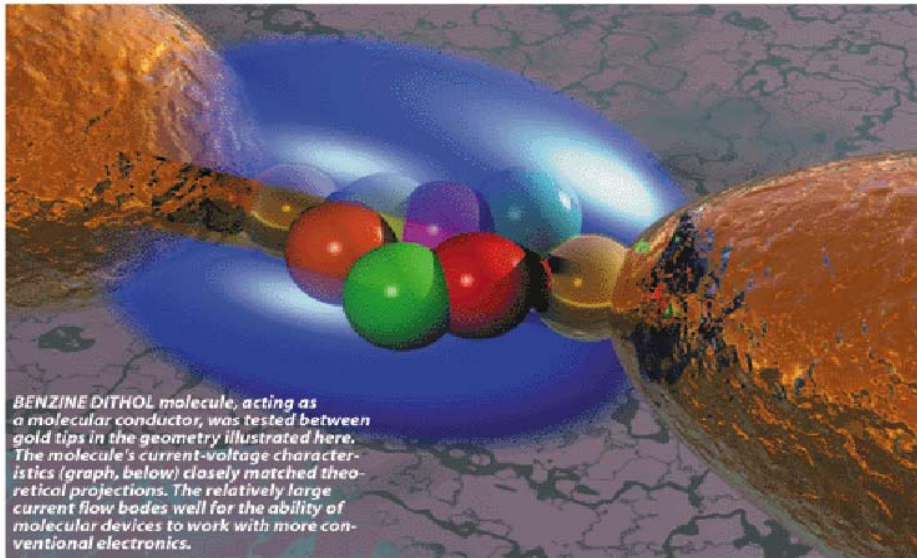
分子电子学和光子学的 多尺度理论研究

江俊

中国科学技术大学

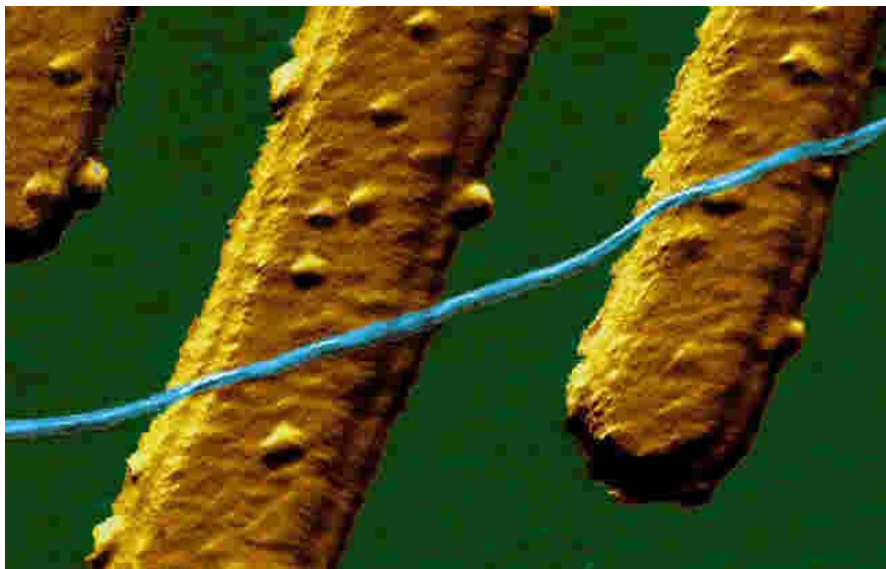
分子电子学：分子科学与电子信息学科交叉，基于分子体系进行电子信息处理，或应用电子学理论技术研究分子科学问题。



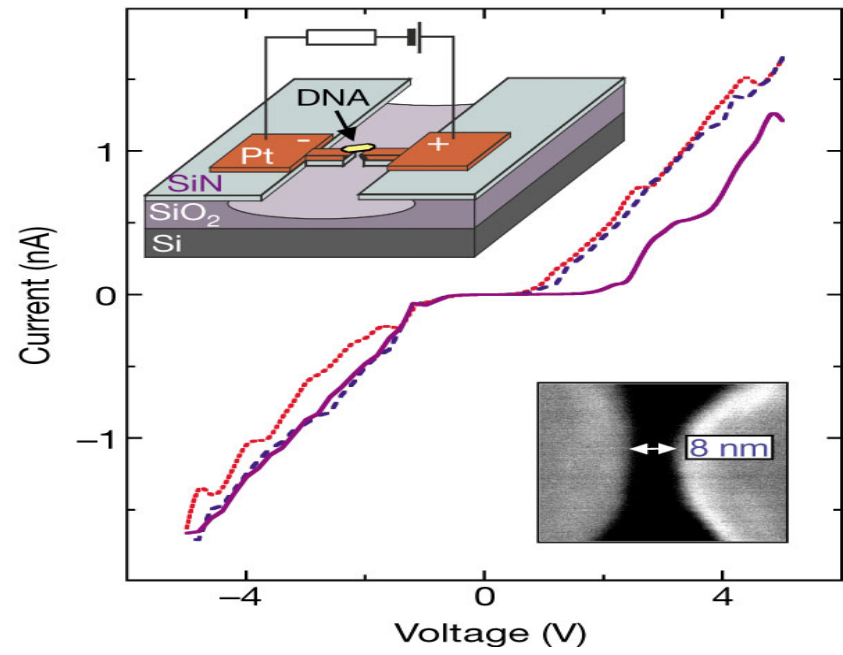


Mark A. Reed and James M. Tour, Scientific American (June '00)

FET



SWCNT across Pt Electrodes (C. Dekker, Delft)



分子电子学：用分子（纳米尺度）作为基本单元进行信息信号处理

➤ **Size: scale from 1 to 100 nm**

Given the same amount of space, many times faster and more powerful than silicon based devices

➤ **Manufacturing:**

- fabricated identically and defect-free in enormous numbers
- Self-assembly Manufactured
- molecular synthesis tools highly developed

➤ **Quantized electron energy**

➤ **Extended π systems**

- Provides thermodynamically favorable electron conduction
- π Conjugation acts conduction switch

➤ **Elegance**

Elegant solutions to non-volatile and inherently digital

研究背景

The problems of chemistry and biology can be greatly helped if our ability to see what we are doing, and to do things on an atomic level, is ultimately developed — a development which I think cannot be avoided.

Richard Feynman

随着近年来纳米和光谱技术的飞跃发展，从原子和分子的微观角度来理解和指导功能材料与器件的研究已表现出明显优越性。

研究背景

- 纳米尺度的观察和调控技术的发展为理论化学研究带来了巨大的机遇
- 理论化学主要是运用数学、物理和计算方法来研究分子和原子的化学现象与体系。
- 上世纪30年代发展的量子力学原理引发了物理学、化学、电子学领域的技术革命，随之确立的固体物理理论指引了现代微电子信息技术的繁荣发展。
- 近年来，量子化学理论方法和计算技术在突飞猛进，人们从原子和分子的微观角度来理解材料器件的能力也大大提高

研究背景

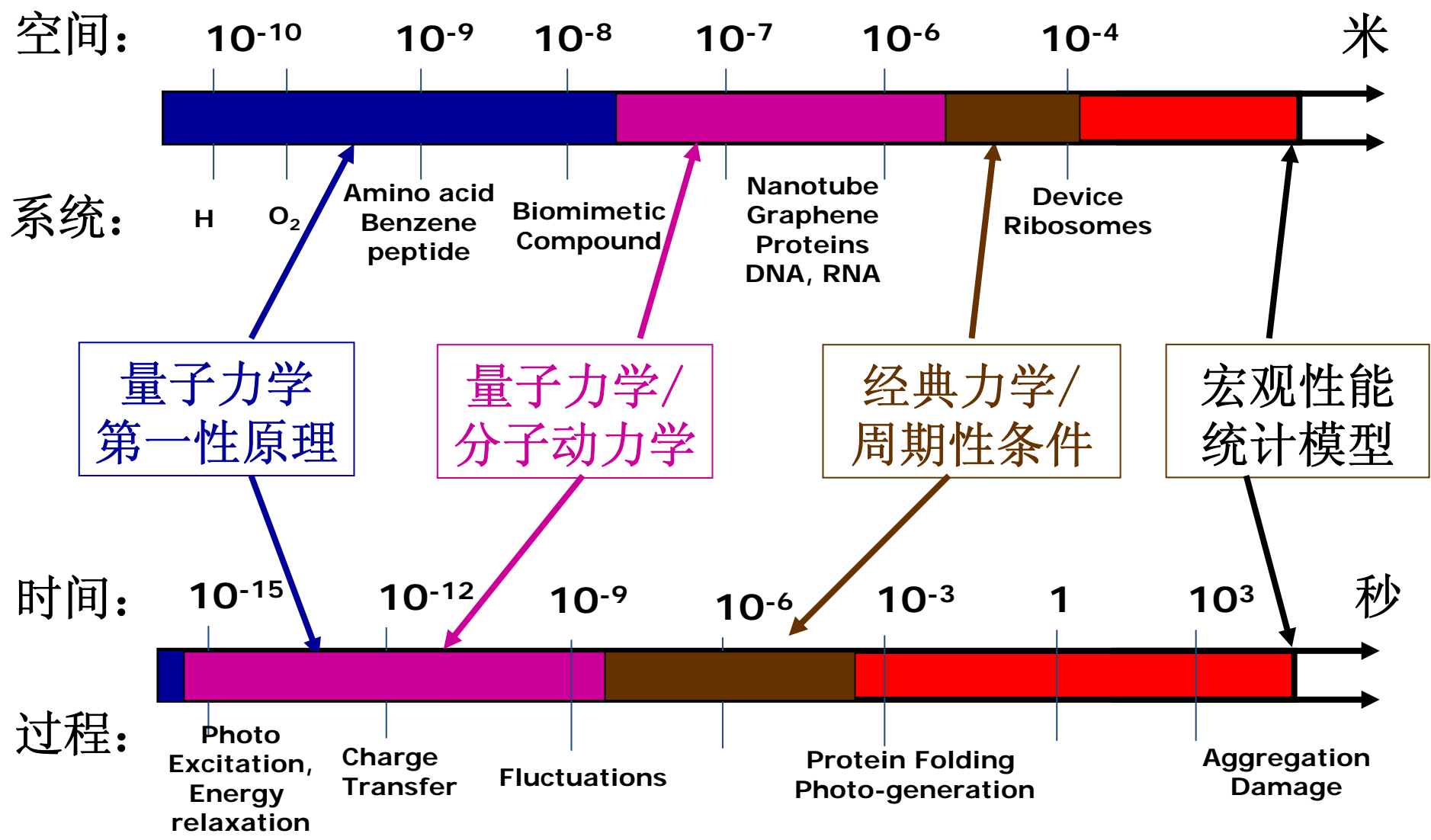
The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

Paul. A. M. Dirac

真实体系的复杂性也为理论化学研究带来了巨大的挑战，例如纳米材料与生物大分子的结构与机理过程的空间与时间尺度分布很广，而这些不同尺度适用于不同的理论方

发展多尺度的理论框架

分子体系的空间和时间尺度复杂性给理论模拟带来巨大挑战!



多尺度理论模拟

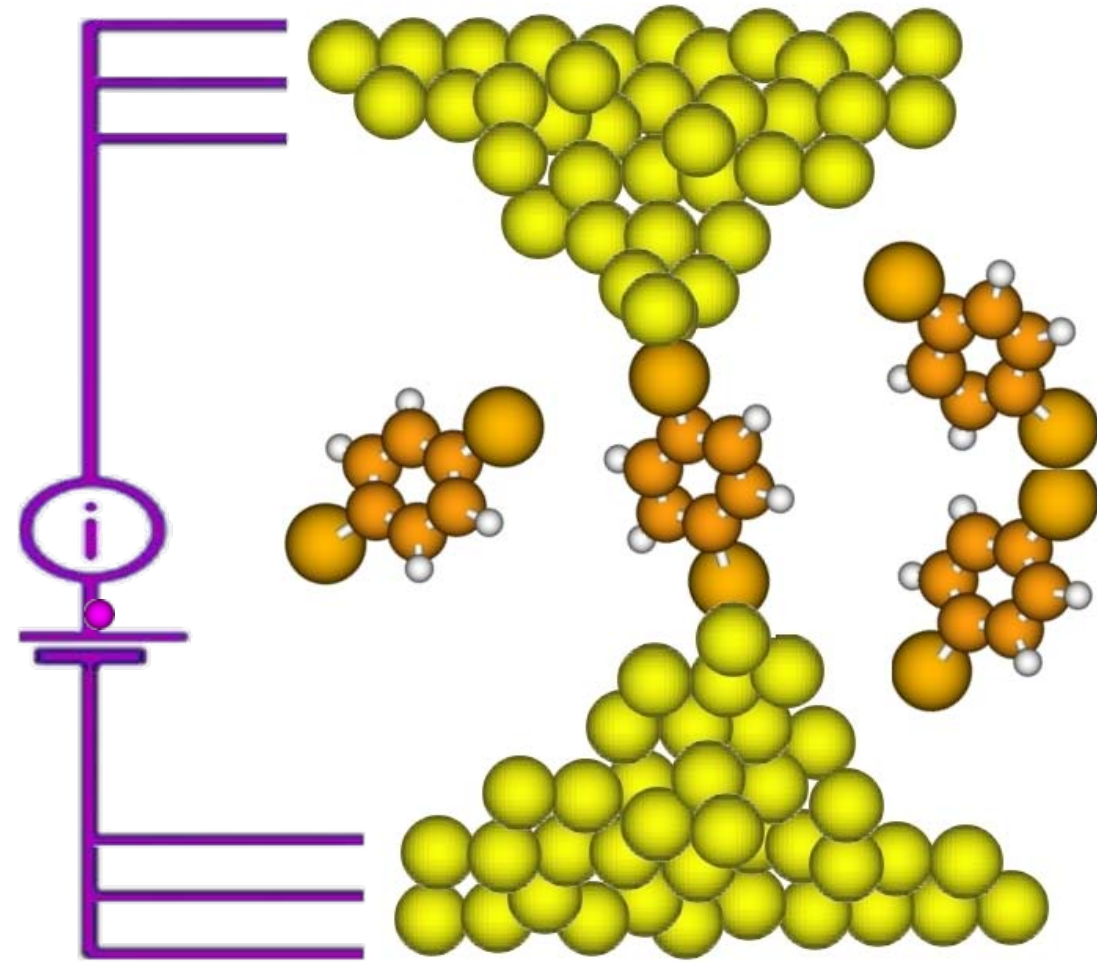
- 针对真实体系的复杂性，灵活动态结合量子化学、分子动力学、固体物理、统计数学等方法，模拟各种空间和时间尺度下的系统和效应
- 集成微观机理构筑宏观图像，提供真实体系结构、功能和机理等关键信息
- 通常从量子化学、固体物理、分子动力学、统计数学，模拟精度和计算所耗资源依次下降，保持精度与效率的平衡

多尺度方法模拟分子器件

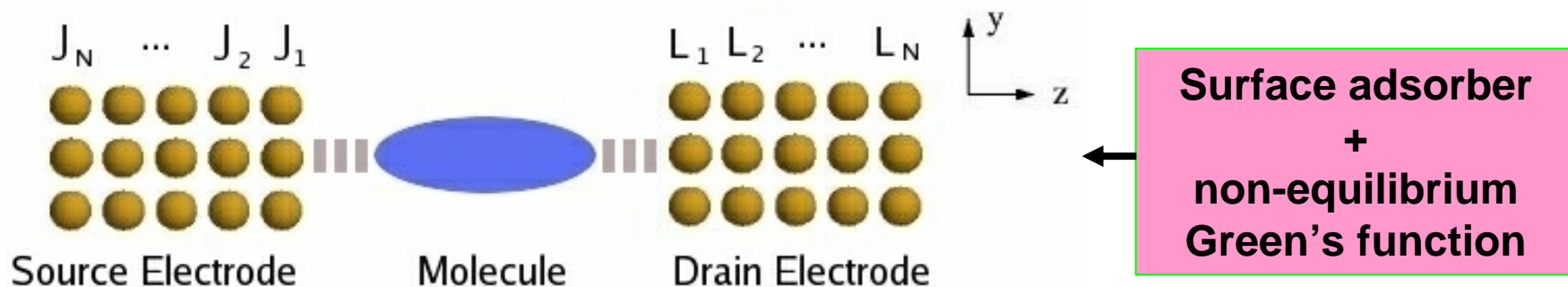
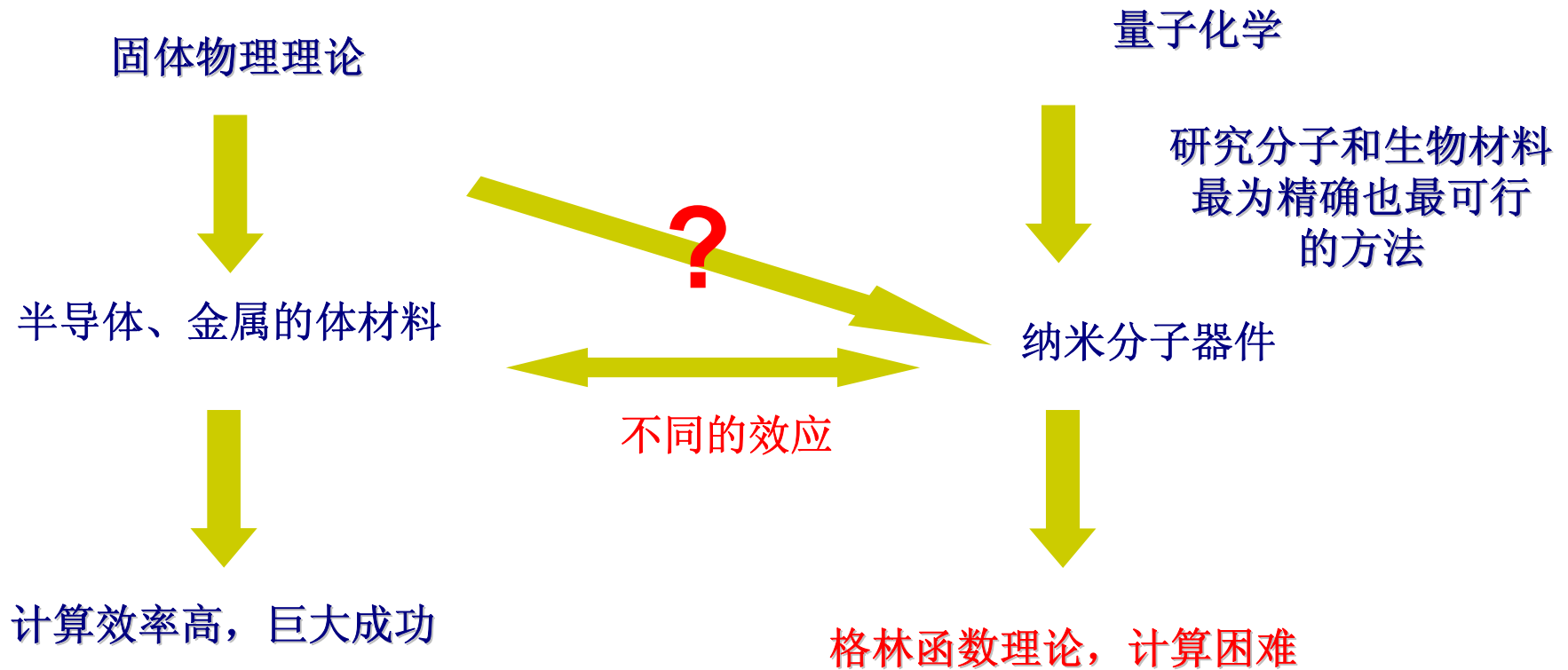
我们的工作:

- 结合固体物理理论（处理微米尺度金属电极）和量子化学计算（描述纳米尺度分子结），模拟分子器件，发展分子电子学理论方法
- 开发独立的软件包QCME (Quantum chemistry for molecular electronics)
- 提出新的电子输运机理，解释新的实验现象。

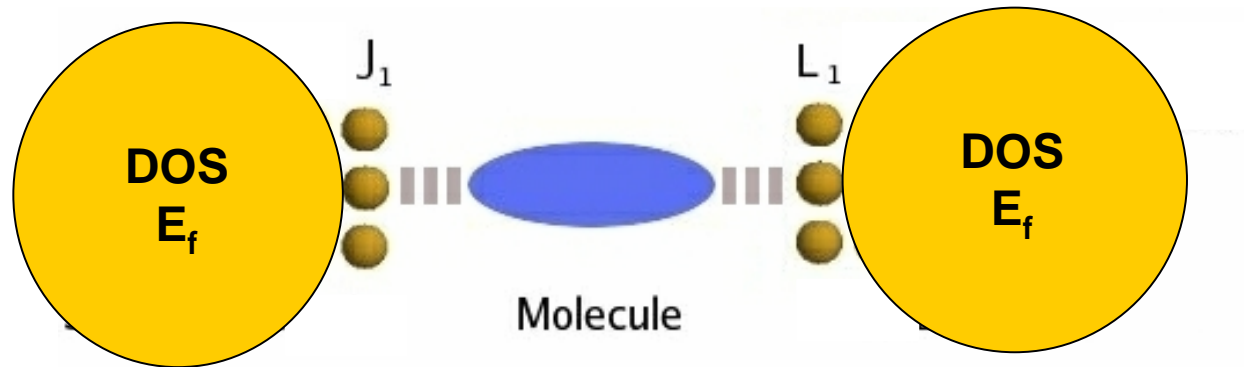
分子器件工作机理



分子电子学理论研究途径



Landauer Formula

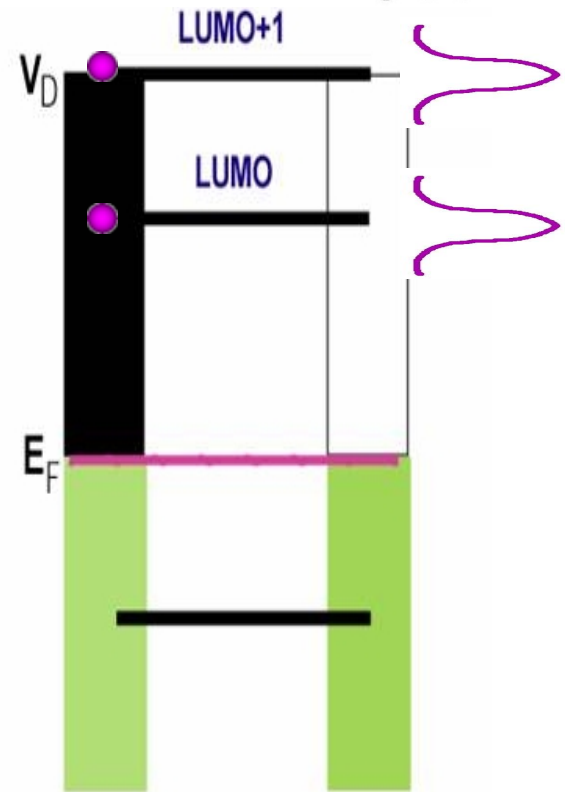
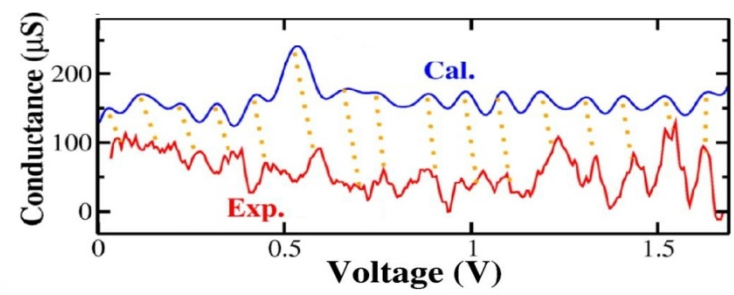
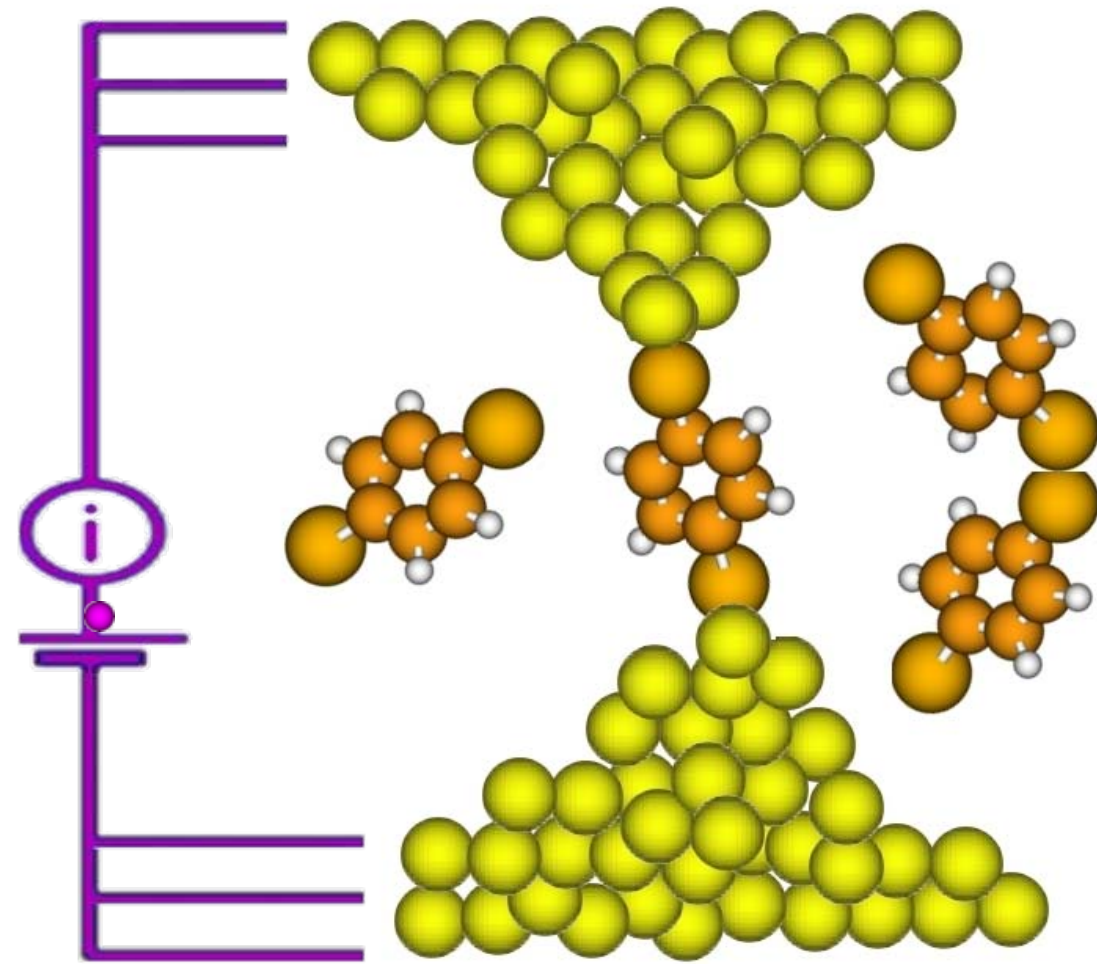


- Treat the “extended molecule” with Quantum Chemistry
- Describe the electrode with Density of States (DOS)
- The extended molecule is in equilibrium with the source and drain by lining up the effective Fermi level

Tunneling Current Density from Source to Drain:

$$\frac{2\pi}{\hbar} \sum_{k,q} T \times f(E_k) \times [1 - f(E_q)] \times \delta(E_k - E_q)$$

分子器件工作机制



多尺度模拟处理大尺寸纳米系统

我们的工作:

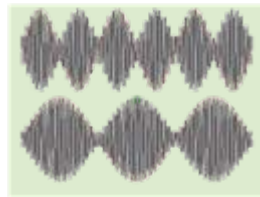
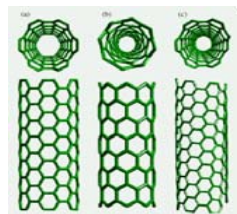
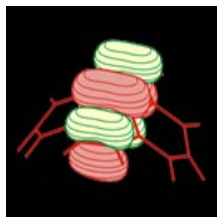
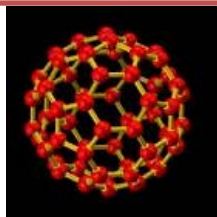
- 发展中央插件延长法 (CIS: Central Insertion Scheme), 有效处理有边界的纳米准周期系统
- 连接小分子(量子化学)和延展体系(固体物理)两个不同尺度及其适用理论
- 开发独立软件包BioNano-Lego
- 解释实验现象, 发掘机理, 提出新的分子设计方案

纳米材料的理论模拟

基于第一性原理的计算方法

量子化学方法

固体物理方法



少于一千个电子的有限分子系统
原子和分子尺度的电荷分布

有边界的纳米准周期系统——没有合适的方法！

无限的周期系统
平面波形式的周期性波函数

Multi-scale Method (多尺度方法)

A straightforward method can be interfaced with quantum chemistry approach

Allows to effectively treat very large nano-scale periodical systems without losing the accuracy

Electronic structure was obtained by solving the Schrodinger Equation

$$H | \Psi^\eta \rangle = \varepsilon_\eta | \Psi^\eta \rangle$$

- Energy of electrons can be written as $\langle \Psi | \hat{H} | \Psi \rangle$
- By the *variational theorem*, this is an upper bound on the true electronic ground state energy
- We minimise the electronic energy as a function of weighting functions of molecular orbitals to obtain *self-consistent* solution (also called SCF approach)
- Use a linear combination of orbital basis functions, or sometimes Gaussian functions:

$$\Psi_i = \sum_{\mu=1}^N C_{\mu i} \phi_\mu \quad \text{LCAO}$$

- Substituting these into a 1-electron T.I. Schrödinger eq.:

$$f \Psi_i = \varepsilon_i \Psi_i \rightarrow f \sum_{\mu=1}^N C_{\mu i} \phi_\mu = \varepsilon_i \sum_{\mu=1}^N C_{\mu i} \phi_\mu$$

Fock Matrix

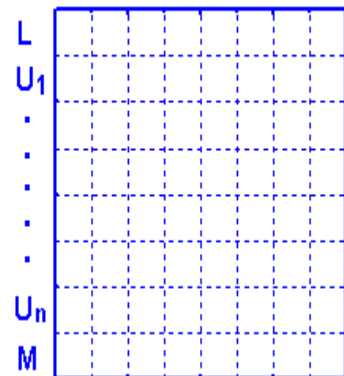
- The hamiltonian of the system can be described as:

$$H = \begin{pmatrix} H_{1,1} & \dots & H_{1,\frac{n}{2}} & H_{1,\frac{n}{2}+1} & \dots & H_{1,n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ H_{\frac{n}{2},1} & \dots & H_{\frac{n}{2},\frac{n}{2}} & H_{\frac{n}{2},\frac{n}{2}+1} & \dots & H_{\frac{n}{2},n} \\ H_{\frac{n}{2}+1,1} & \dots & H_{\frac{n}{2}+1,\frac{n}{2}} & H_{\frac{n}{2}+1,\frac{n}{2}+1} & \dots & H_{\frac{n}{2}+1,n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ H_{n,1} & \dots & H_{n,\frac{n}{2}} & H_{n,\frac{n}{2}+1} & \dots & H_{n,n} \end{pmatrix}$$

where F is the *Fock* n

S is the *overlap matrix*

The equation can be



exactly in matrix form :

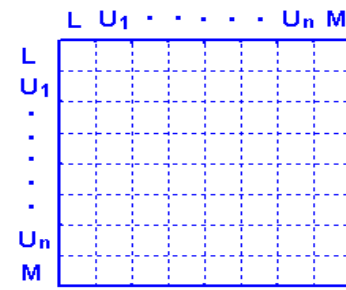
$$\mathbf{FC} = \mathbf{SC}\boldsymbol{\varepsilon}, \text{ or,}$$

all equations

$$(\mathbf{F} - \mathbf{S}\boldsymbol{\varepsilon})\mathbf{C} = 0$$

n)

The most resource consuming part in Quantum Chemistry calculation is to obtain Fock Matrix through SCF solution



- molecular orbital coefficients C_i that minimise the energy and give us the best single determinant
- In the secular equation, the Fock matrix itself depends on the coefficients C_i , and therefore it is necessary to use an iterative procedure when solving the equation
- We guess values for the C_i initially and the variational principle (which states that E_{guess} is always $> E_{\text{true}}$) allows us to optimise the C_i until we reach self-consistency
- However, the Fock matrix contains many two-electron integrals which are very time-consuming to calculate

中央插件延长法(Central Insertion Scheme)

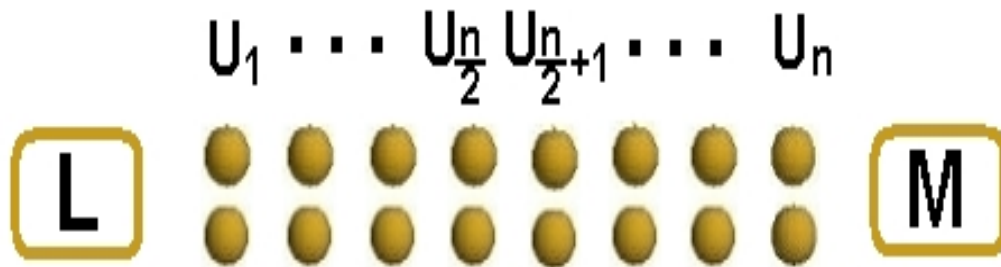
Deduce out the Fock matrix of large nano-scale systems from the smaller scale system

Greatly reduce computation time and resource by avoiding the SCF process

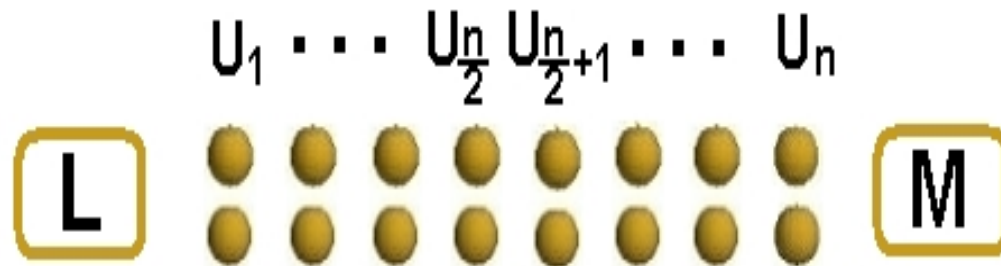
中央插件延长法(Central Insertion Scheme)

Approximations:

- 1) periodical short-nano-scale systems are long enough to have the electronic structures converged in the central parts
- 2) long distance interaction ($> 20 \text{ \AA}$) between subsystems dies out in the short-nano-scale systems



1) Electronic structures converged in the core parts



- The hamitonian of the system can be described as:

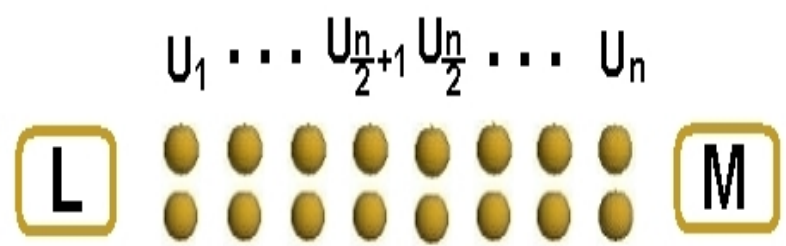
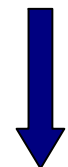
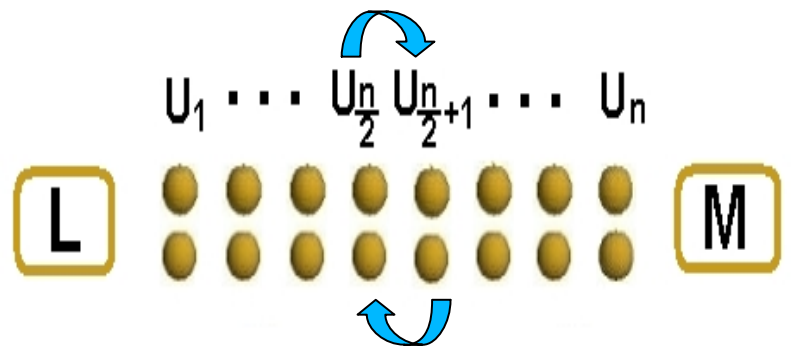
$$H = \begin{pmatrix} H_{1,1} & \cdots & H_{1,\frac{n}{2}} & H_{1,\frac{n}{2}+1} & \cdots & H_{1,n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ H_{\frac{n}{2},1} & \cdots & H_{\frac{n}{2},\frac{n}{2}} & H_{\frac{n}{2},\frac{n}{2}+1} & \cdots & H_{\frac{n}{2},n} \\ H_{\frac{n}{2}+1,1} & \cdots & H_{\frac{n}{2}+1,\frac{n}{2}} & H_{\frac{n}{2}+1,\frac{n}{2}+1} & \cdots & H_{\frac{n}{2}+1,n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ H_{n,1} & \cdots & H_{n,\frac{n}{2}} & H_{n,\frac{n}{2}+1} & \cdots & H_{n,n} \end{pmatrix}$$

- The convergence of interaction

$$H_{\frac{n}{2},\frac{n}{2}} = H_{\frac{n}{2}+1,\frac{n}{2}+1}$$

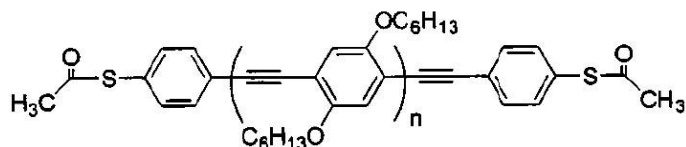
$$H_{\frac{n}{2},\frac{n}{2}+1} = H_{\frac{n}{2}+1,\frac{n}{2}+2}$$

1) Electronic structures converged in the core parts



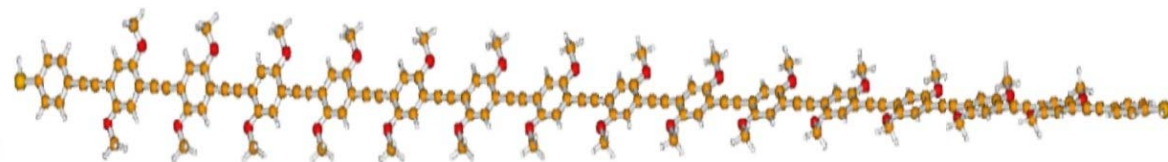
$$H_{\frac{n}{2}, \frac{n}{2}} \longleftrightarrow H_{\frac{n}{2}+1, \frac{n}{2}+1}$$
$$H_{\frac{n}{2}, \frac{n}{2}+1} \longleftrightarrow H_{\frac{n}{2}+1, \frac{n}{2}}$$

Take polymer (n=10) as an example:



$$H_{\frac{n}{2}, \frac{n}{2}} \longleftrightarrow H_{\frac{n}{2}+1, \frac{n}{2}+1}$$

$$H_{\frac{n}{2}, \frac{n}{2}+1} \longleftrightarrow H_{\frac{n}{2}+1, \frac{n}{2}}$$



Gaussian03 computed HOMO(highest occupied orbital)-LUMO(lowest unoccupied orbital) gap: 2.784eV

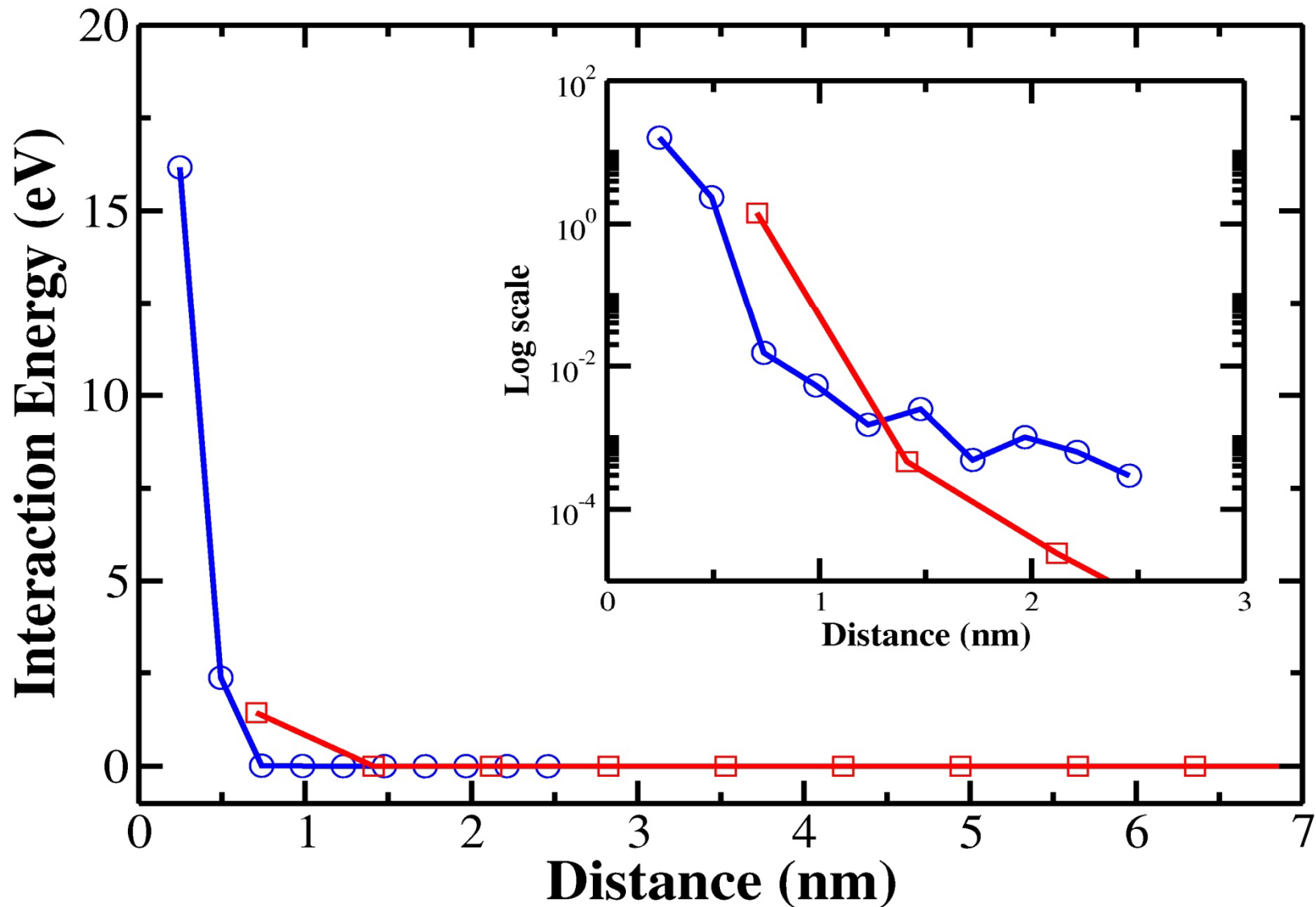
Reconstructing computed HOMO-LUMO gap: 2.786eV, error **2 meV**

Orbital energy error in the range of (HOMO-20, LUMO+20):

Biggest error **8 meV** smallest error **0.0005meV**

electron density	Reconstructing results	GAUSSIAN03 Results	error
U ₁	0.0351	0.0357	0.0006
U ₂	0.0766	0.0771	0.0006
U ₃	0.1259	0.1251	0.0008
U ₄	0.1684	0.1657	0.0027
U ₅	0.1901	0.1847	0.0053
U ₆	0.1835	0.1864	0.0028
U ₇	0.1512	0.1550	0.0038
U ₈	0.1041	0.1086	0.0045
U ₉	0.0571	0.0603	0.0032
U ₁₀	0.0227	0.0242	0.0015

2) long distance interaction dies out

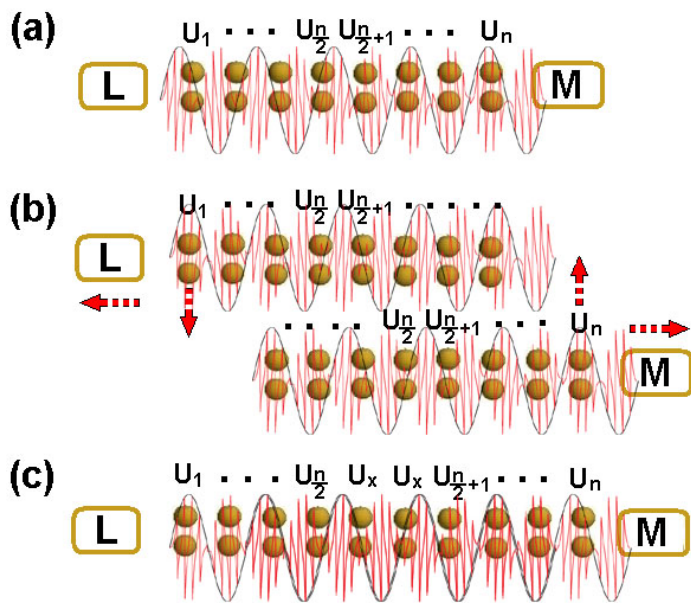


Interaction energy between U1 and other units as a function of distance between them.

Blue Circle dots: CNT21; Red Square dots: POI Y10

发明中央插件延长法显著提高量子化学计算效率!

结构延长



• The hamitonian of the system can be described as:

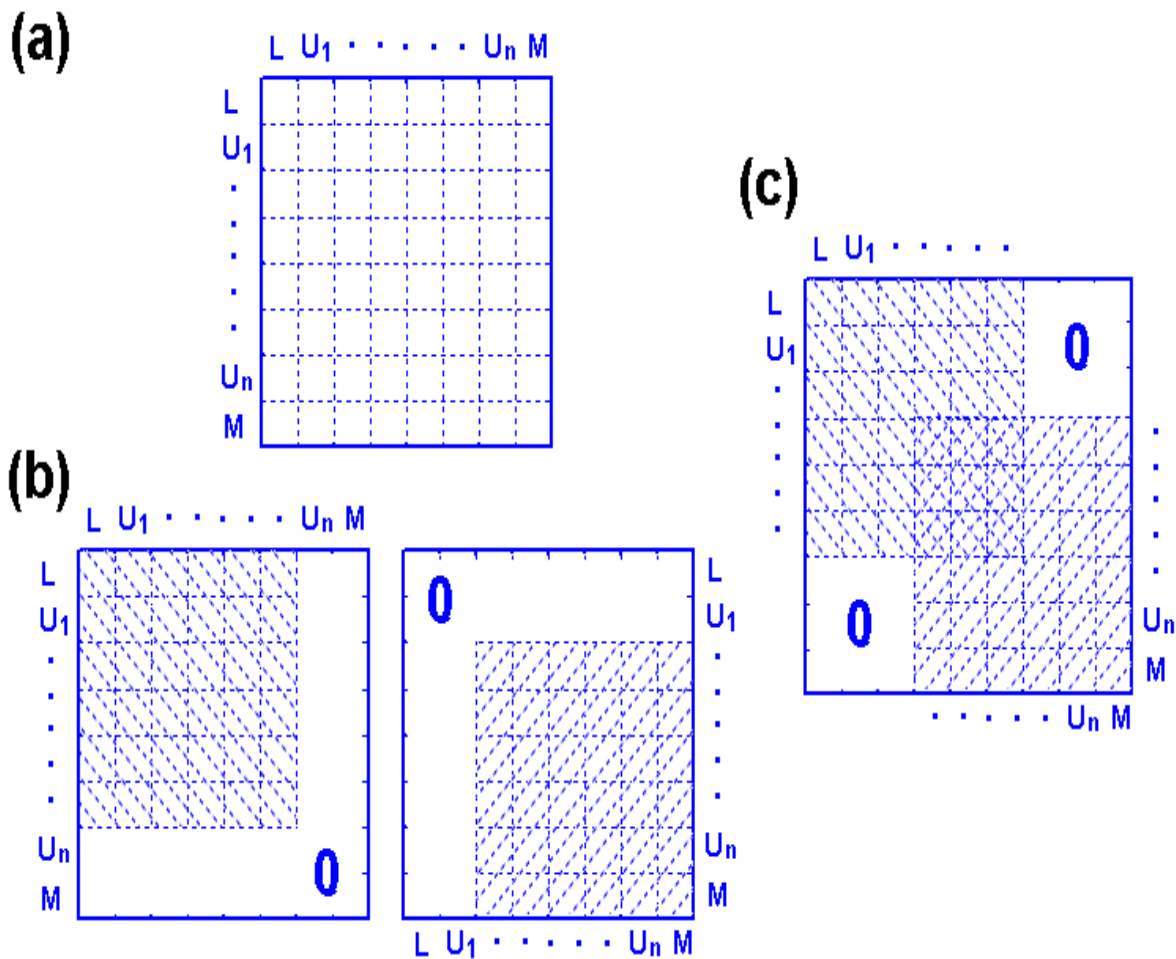
$$H = \begin{pmatrix} H_{1,1} & \dots & H_{1,\frac{n}{2}} & H_{1,\frac{n}{2}+1} & \dots & H_{1,n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ H_{\frac{n}{2},1} & \dots & H_{\frac{n}{2},\frac{n}{2}} & H_{\frac{n}{2},\frac{n}{2}+1} & \dots & H_{\frac{n}{2},n} \\ H_{\frac{n}{2}+1,1} & \dots & H_{\frac{n}{2}+1,\frac{n}{2}} & H_{\frac{n}{2}+1,\frac{n}{2}+1} & \dots & H_{\frac{n}{2}+1,n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ H_{n,1} & \dots & H_{n,\frac{n}{2}} & H_{n,\frac{n}{2}+1} & \dots & H_{n,n} \end{pmatrix}$$

• The convergence of interaction

$$H_{\frac{n}{2},\frac{n}{2}} = H_{\frac{n}{2}+1,\frac{n}{2}+1}$$

$$H_{\frac{n}{2},\frac{n}{2}+1} = H_{\frac{n}{2}+1,\frac{n}{2}+2}$$

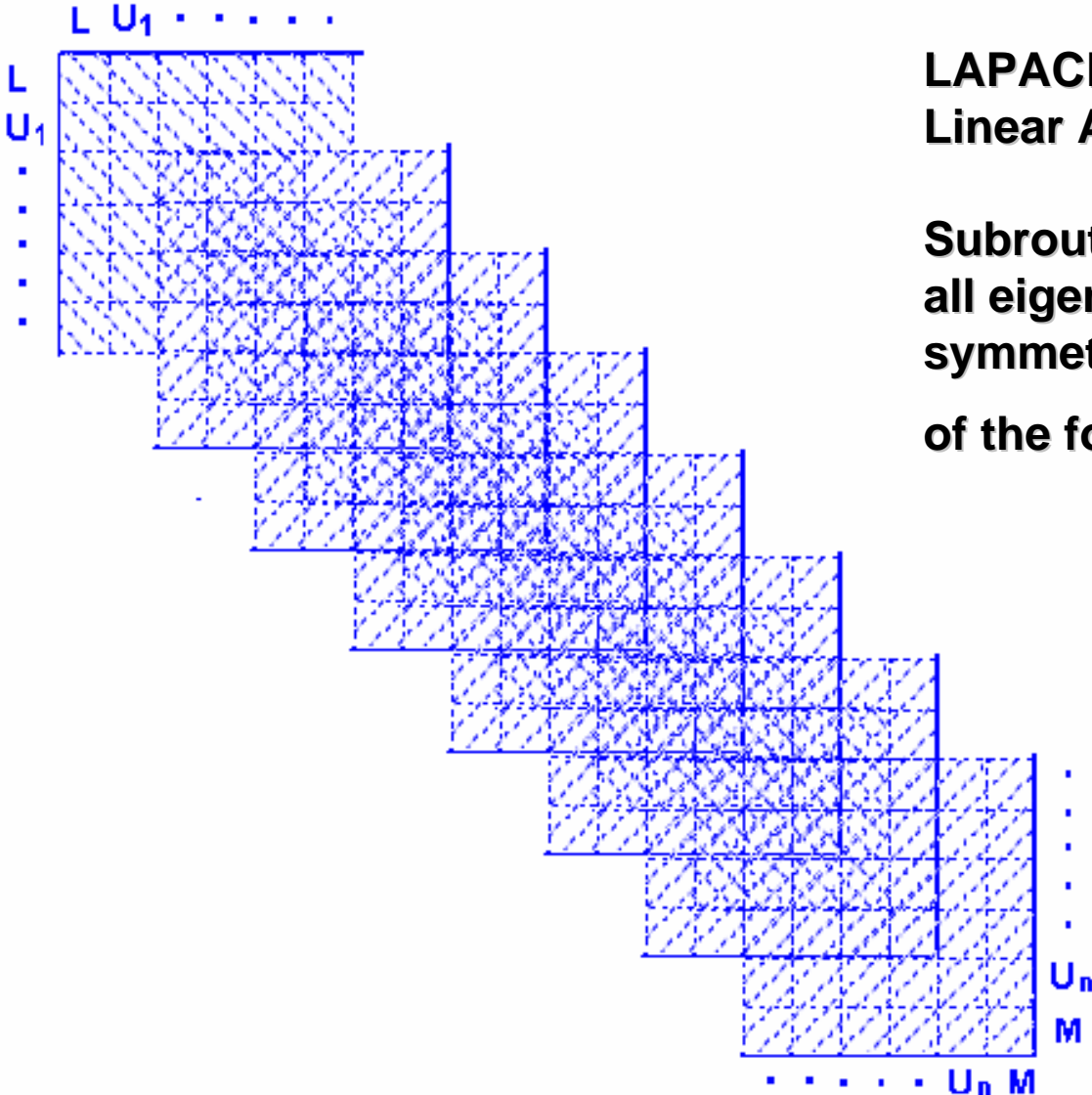
哈密顿矩阵的延长



编写相应软件程序包: Bio-NanoLego

Eigen value solution

For very large scale

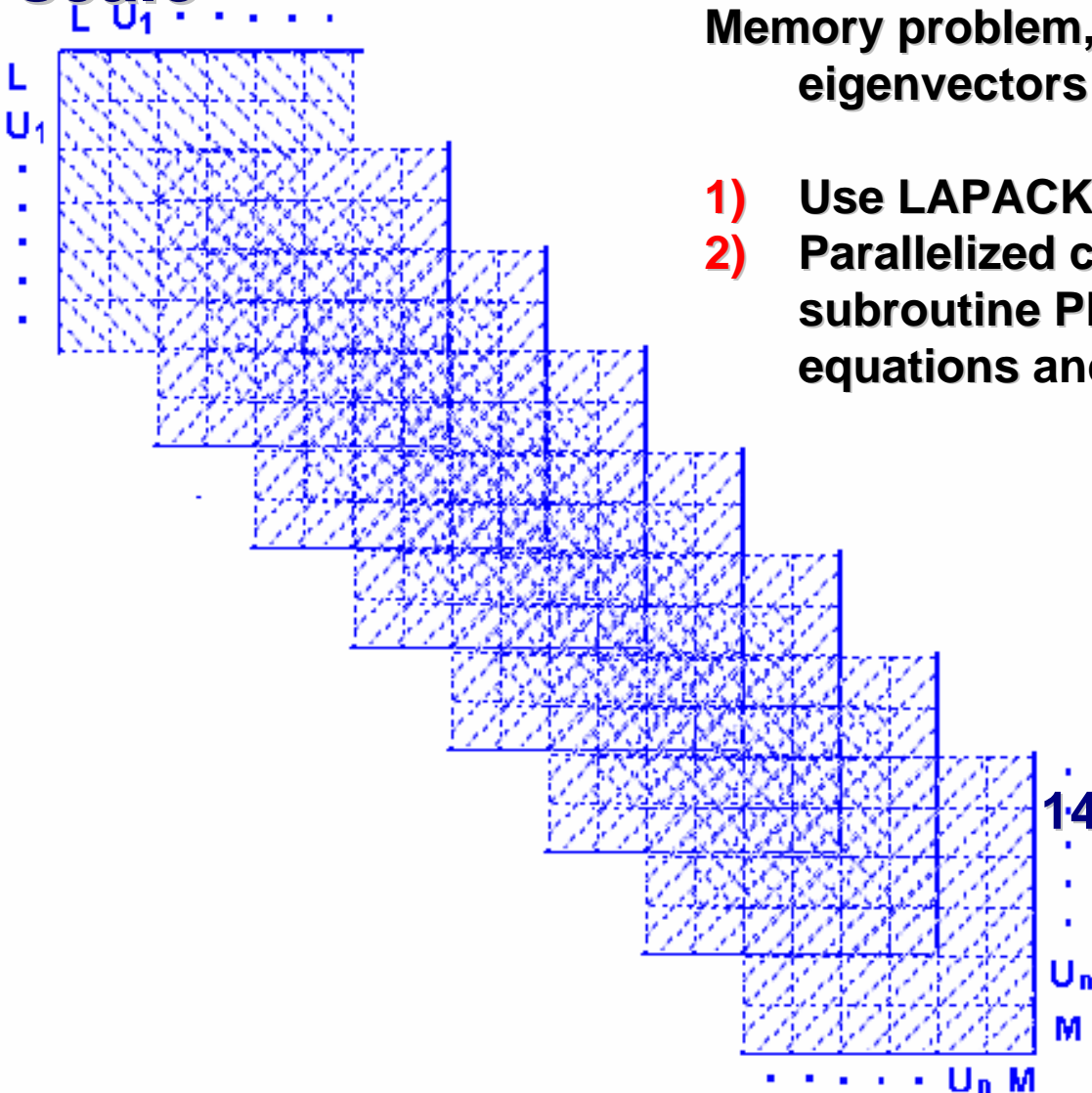


LAPACK –
Linear Algebra PACKage

Subroutine `ssbgv()` or `dsbgv()` Compute all eigenvalues, and eigenvectors of a symmetric-definite banded eigenproblem, of the form $A*x=(\text{lambda})*B*x$

Eigen value solution

For even larger
scale



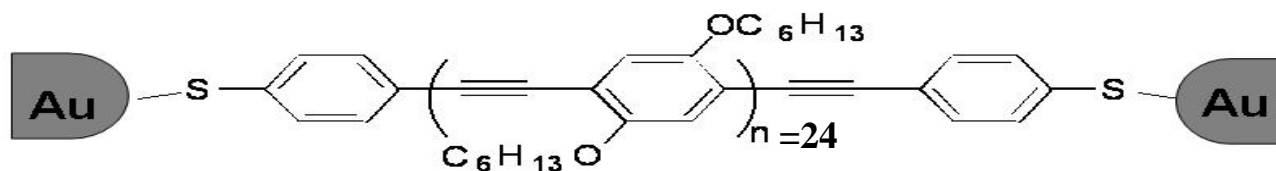
Memory problem, can not find eigenvalues and eigenvectors at the same time

- 1) Use LAPACK Compute all eigenvalues,
- 2) Parallelized calculation with scalapack subroutine PDDBSV to solve the linear equations and find eigenvectors

Biggest system:
200 nm (5 5) carbon nanotube
97, 020 electrons,
145, 570 gaussian basis functions
Maxtrix 145, 570*145,570

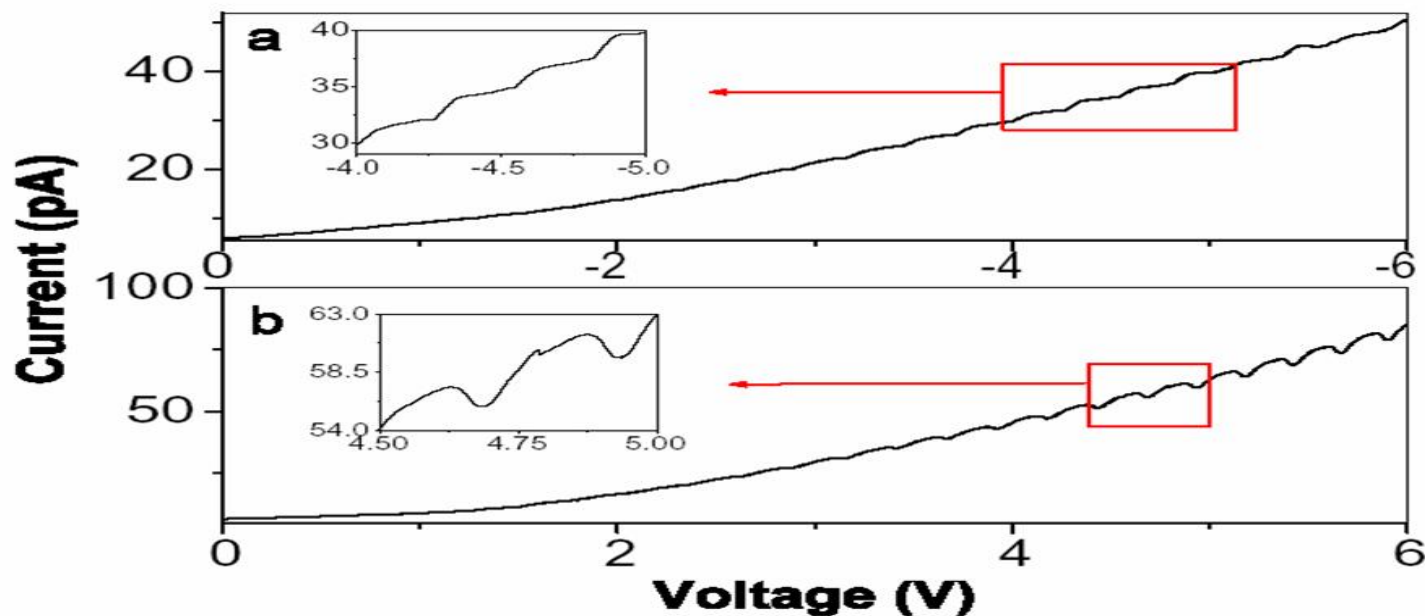
合作者的新实验结果：挑战！

中科院化学所朱道本、胡文平研究组在2005年发现：
18纳米长的共轭分子 (PPE) 具有量子电导效应



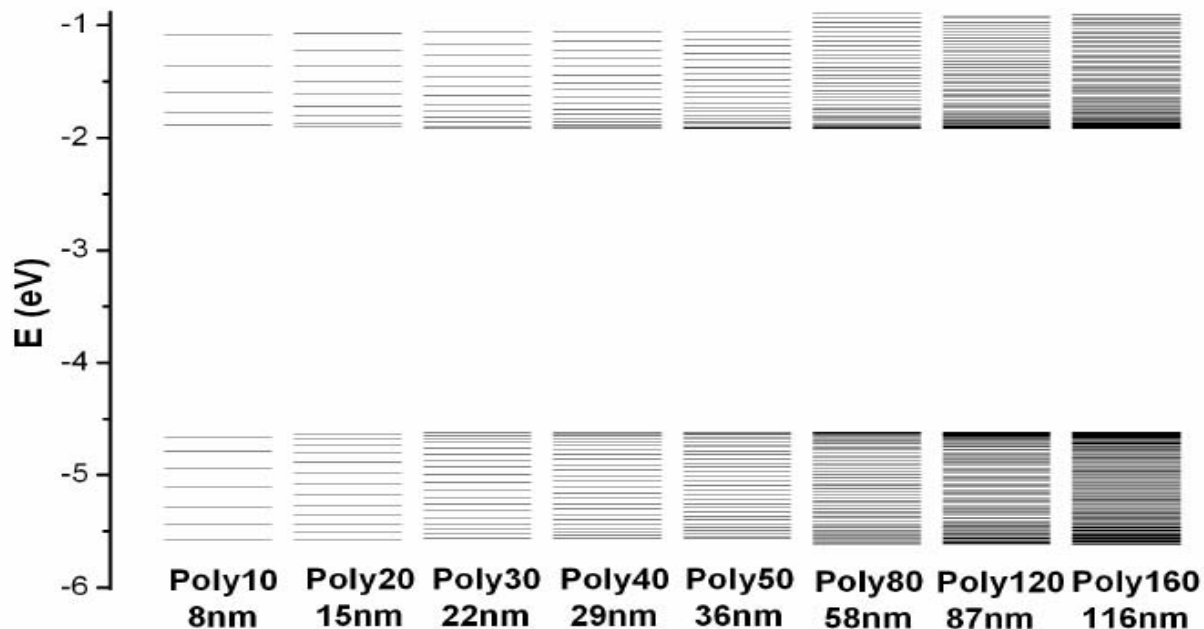
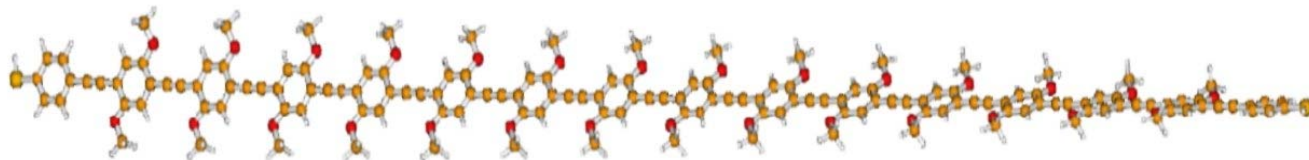
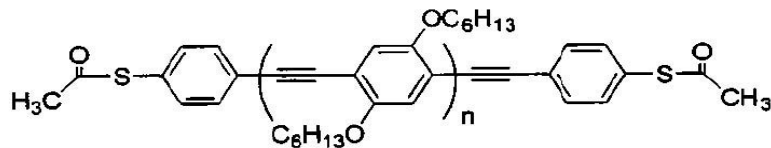
poly(*para*-phenylene ethynylene)s (PP)

Au-Au 距离: 18nm



现有的计算程序包都无法处理如此大的系统!!!

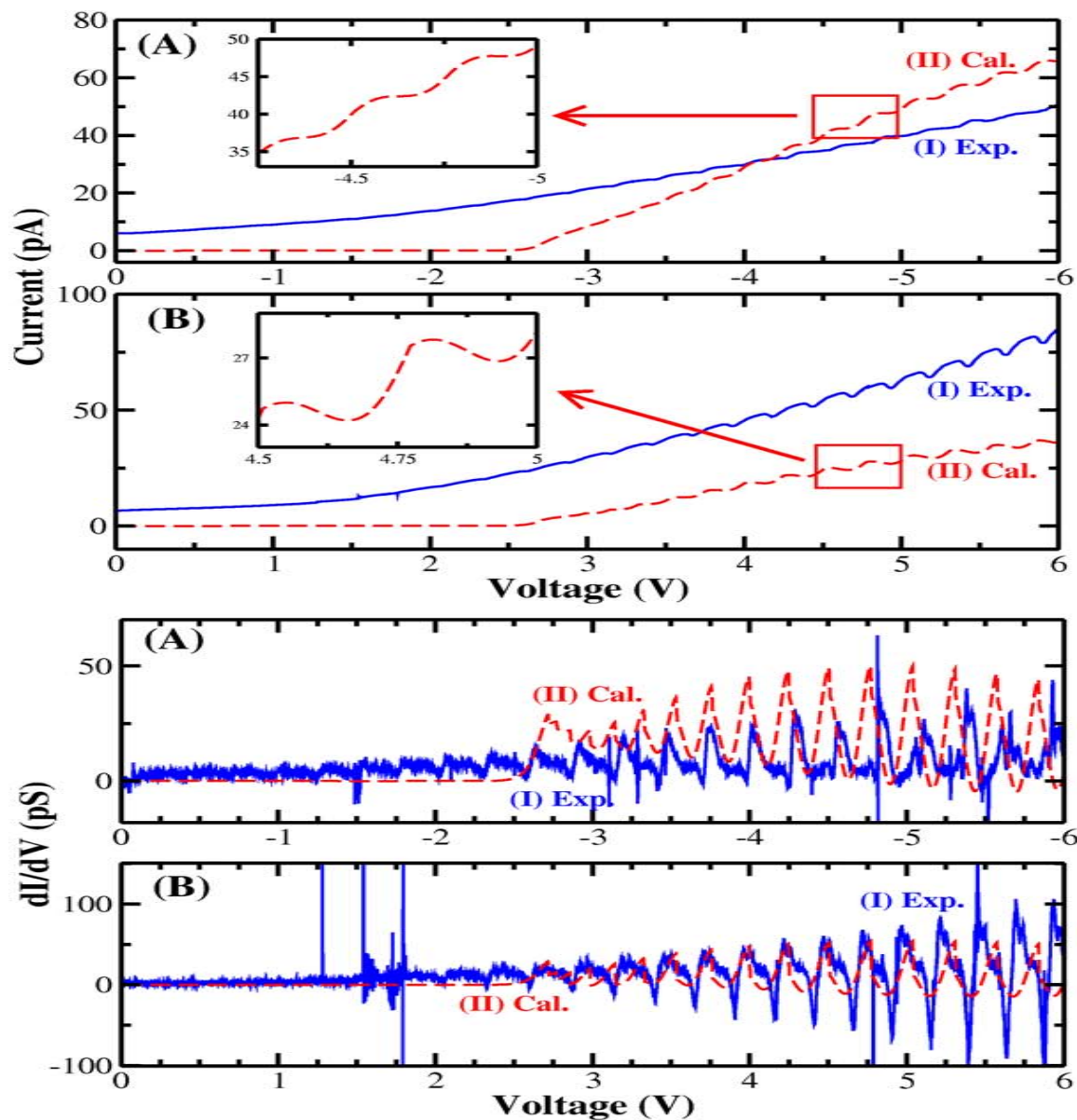
Conjugated Polymer



Increasing of size, Density of State(DOS) increases
Discrete molecular orbital to continuous band
HOMO-LUMO gap remains constant as 2.78eV
Energy structure analogous to inorganic Semiconductor

理论结合实验:

共轭分子PPE (n=24), 18.3 纳米长



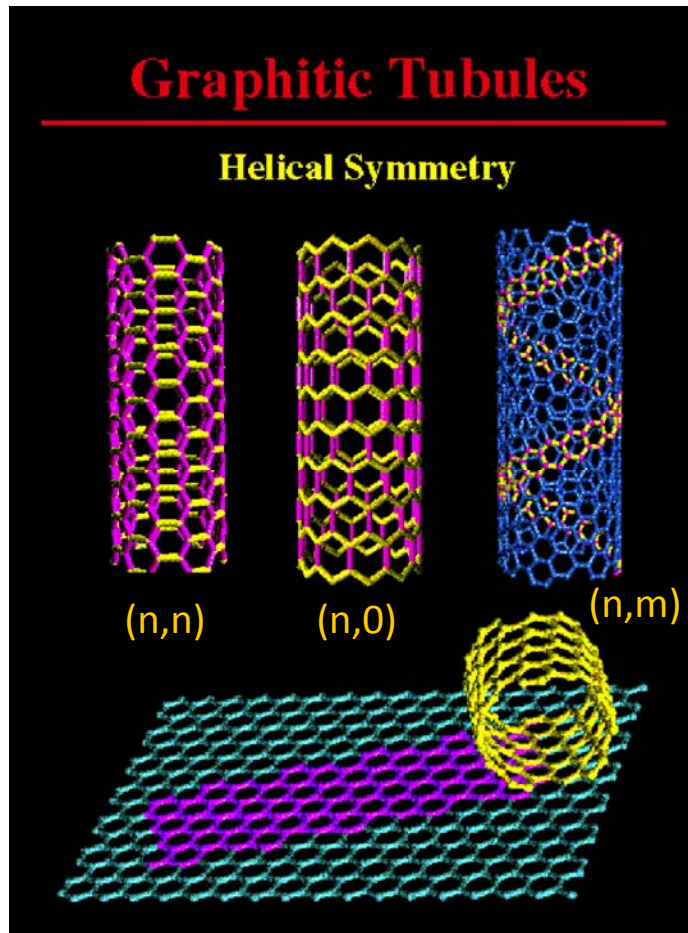
新发现:

如此长的共轭分子的能级结构依然分立

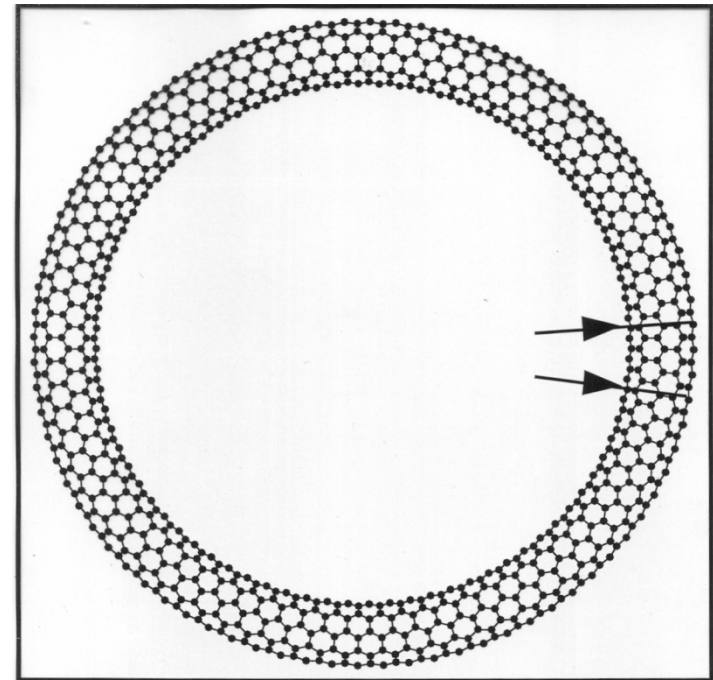
导电过程中起主导作用是弹性电子散射

- **CIS calculation provide accurate electronic structures for very long conjugated polymers**

Carbon Nanotube-based Structures



A Toroidal Carbon Nanotube

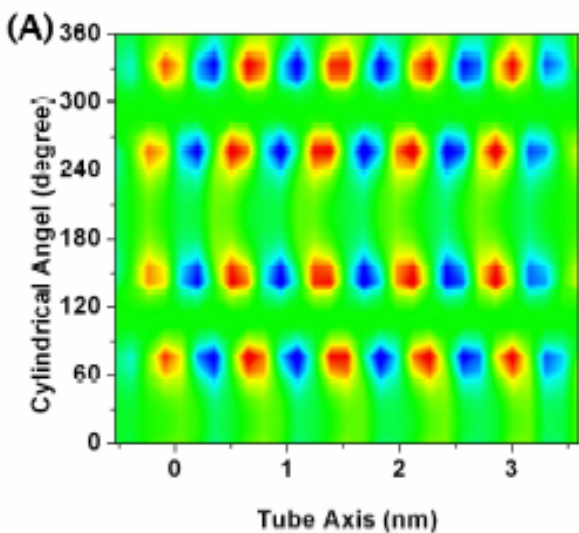
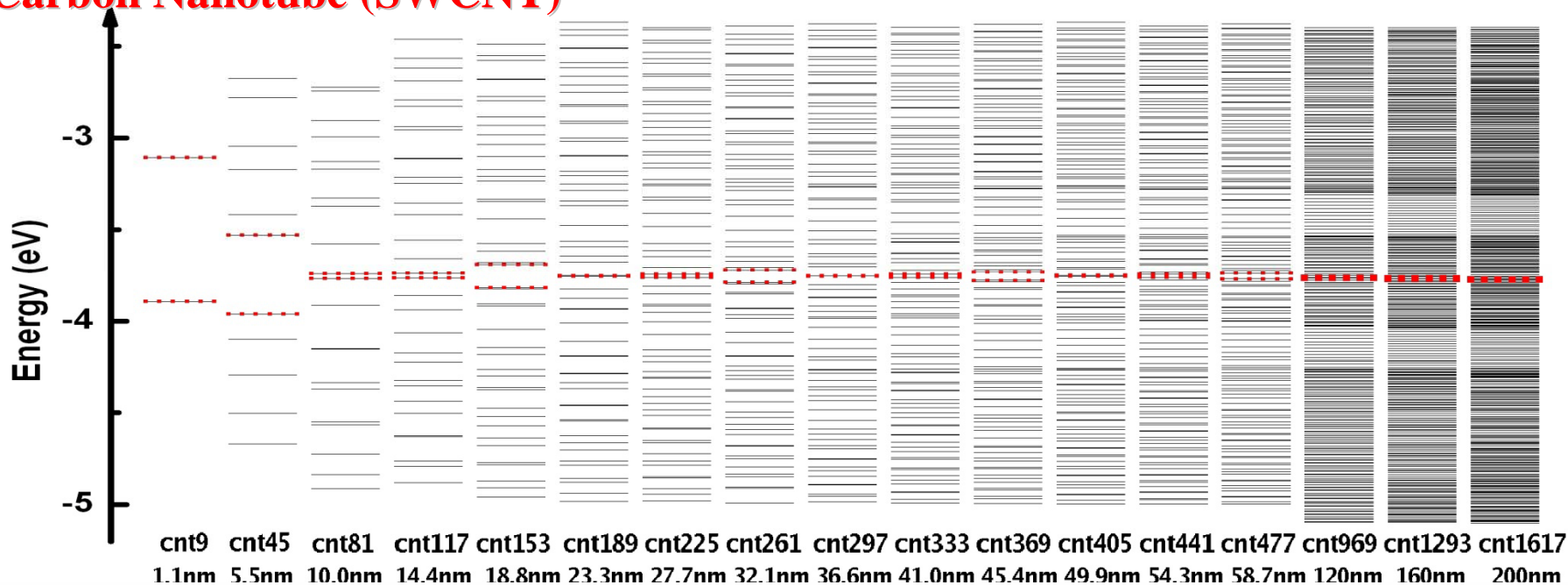


Carbon Nanotubes (CNTs) and toroidal carbon nanotubes (TCNs) are special class of low-dimensional systems which are expected to exhibit novel physical properties due to their special geometries (cylindrical/toroidal) as well as nanoscale sizes

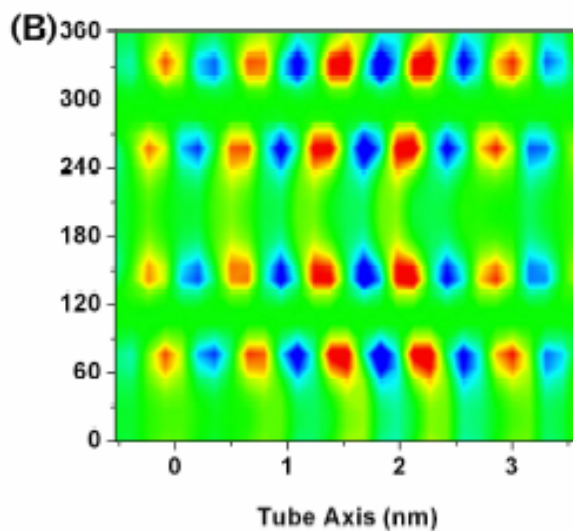
(5, 5) Metallic Single Walled Carbon Nanotube (SWCNT)

B3LYP/6-31G

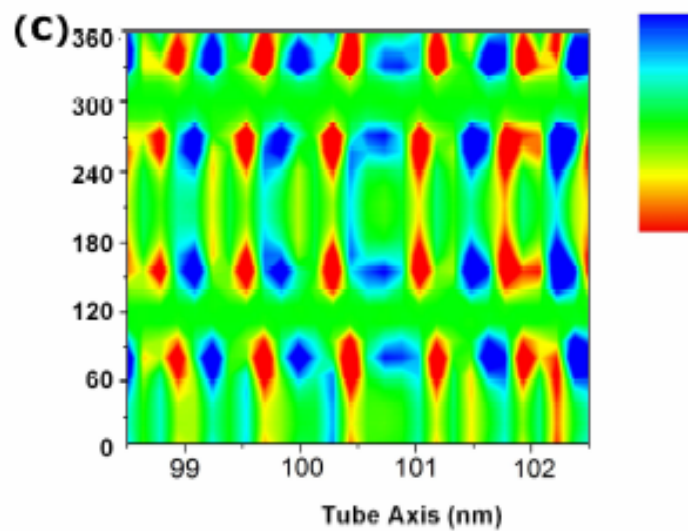
Max: 16170 C atoms described by 150, 000 Gaussian Basis



G03 LUMO of 4.1 nm SWCNT

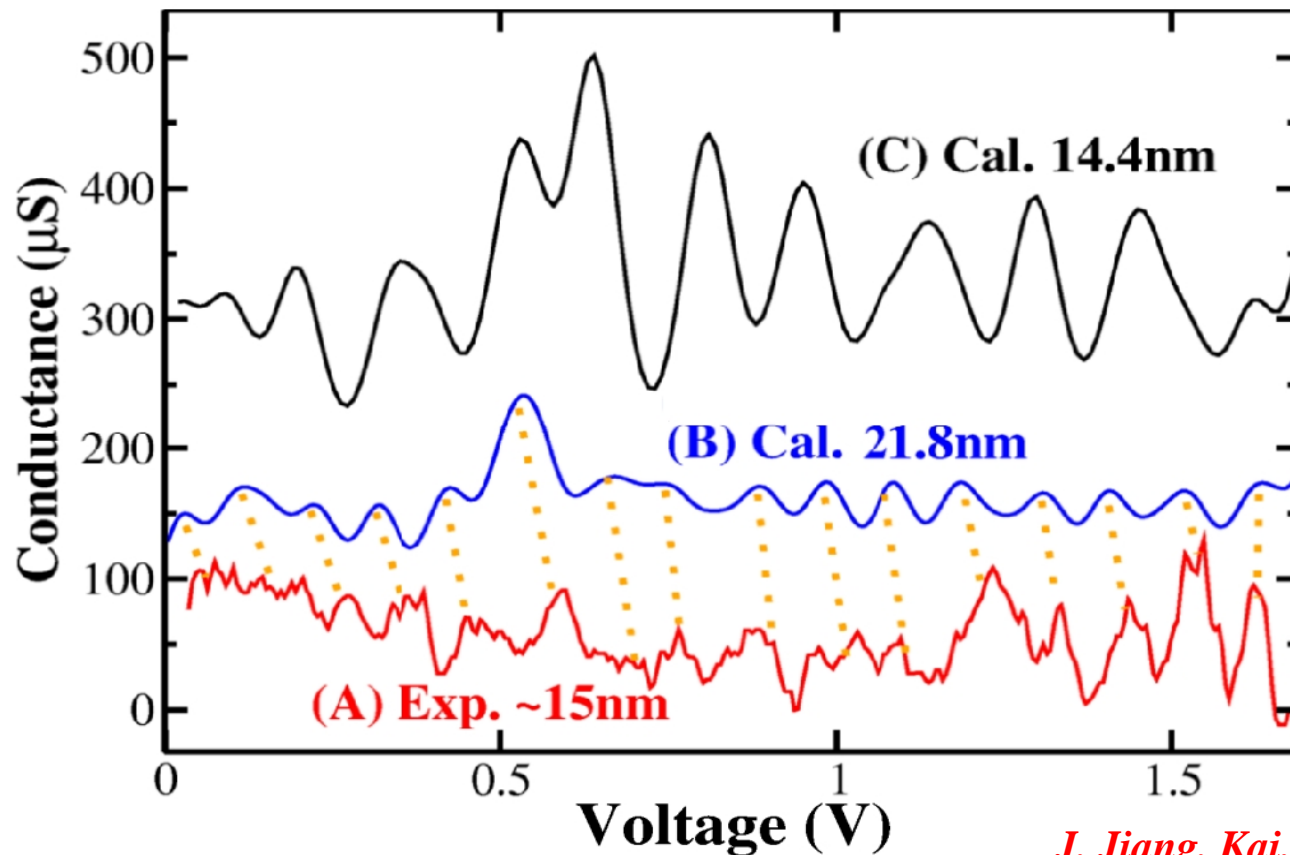
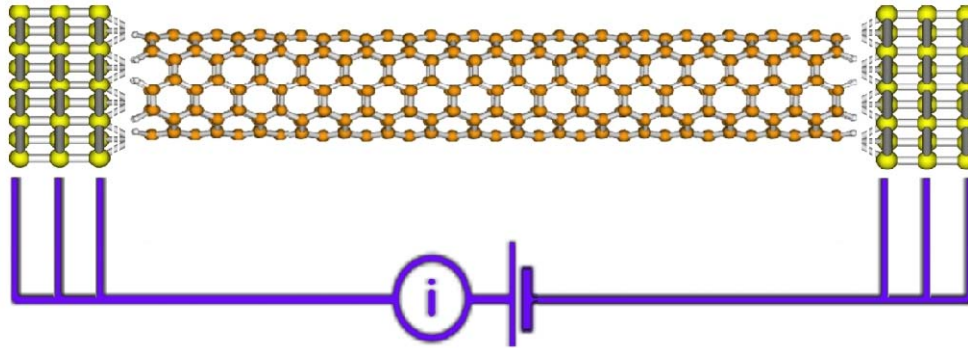


CIS LUMO of 4.1 nm SWCNT



CIS LUMO of 200 nm SWCNT

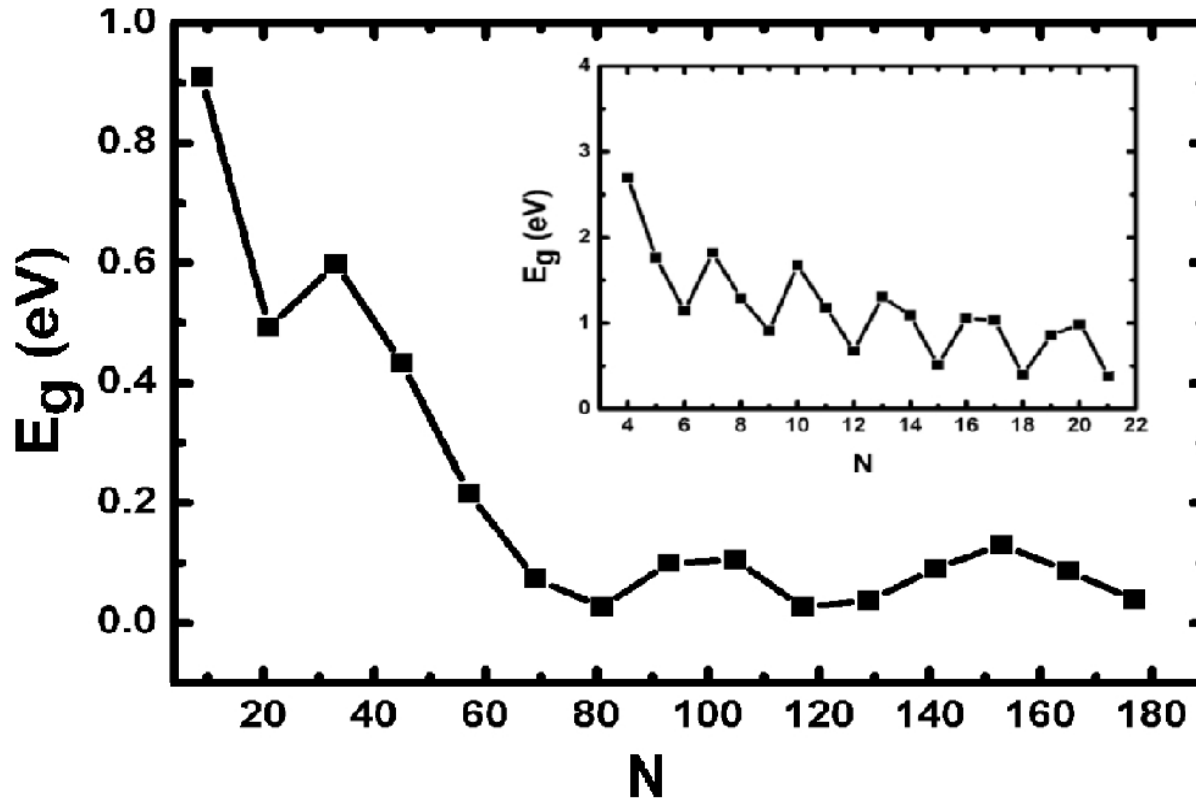
Electron transport in (5, 5) CNT



*J. Jiang, Kai.Liu, Y. Luo,
J. Chem. Phys. 124, 214711. 2006*

[Exp: Javey et al. PANS, 101 \(2004\) 13408](#)

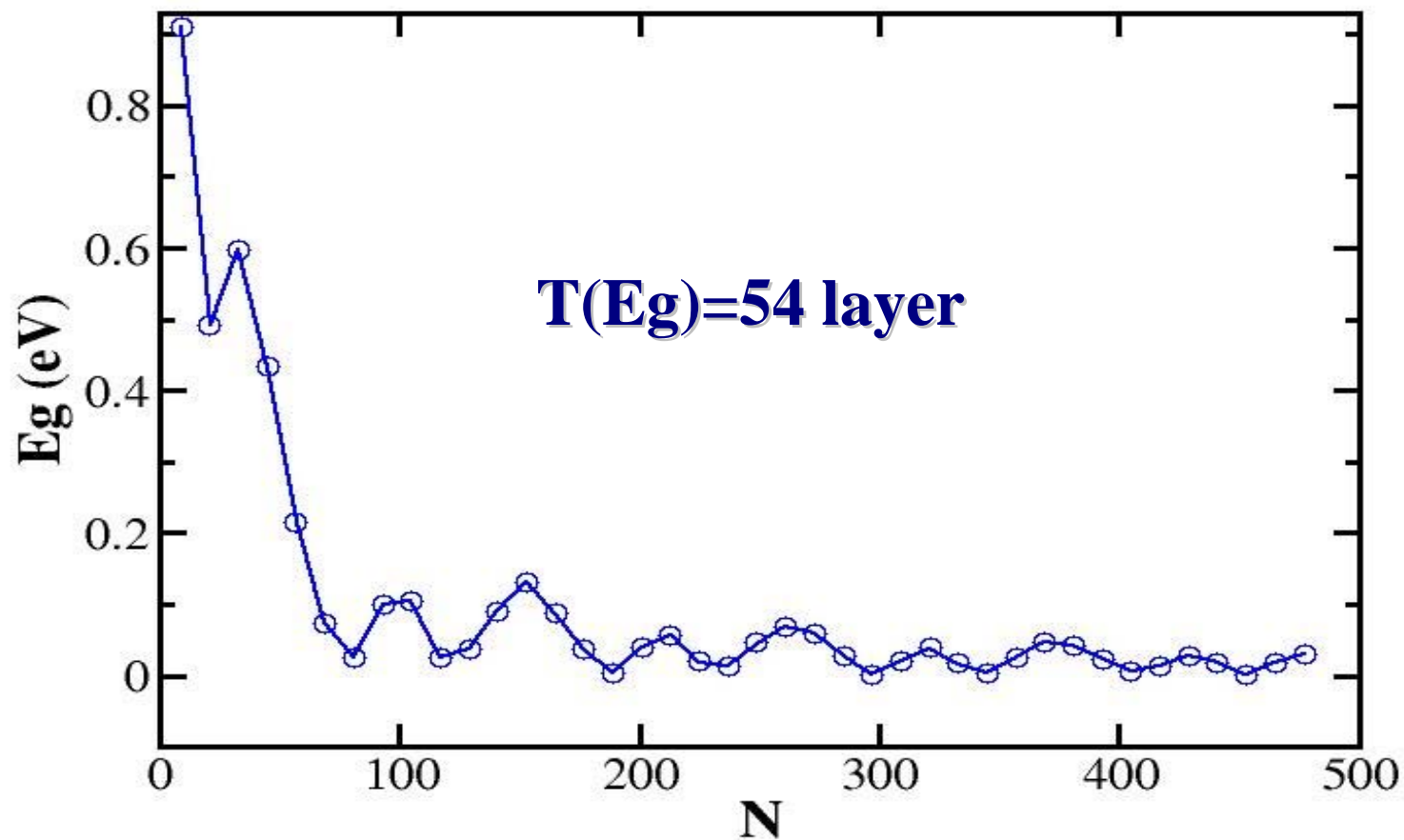
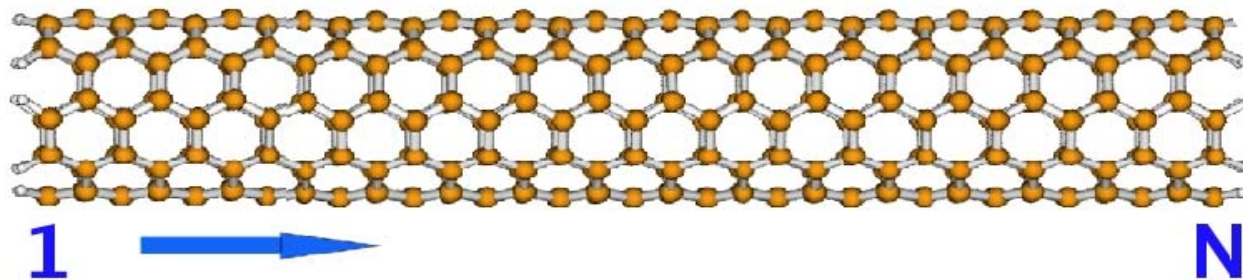
(5, 5) metallic CNT



Bigger-period oscillation superimposed on the 3 units period oscillation:
Interference effect between the one dimensional quantum confinement along the tube direction and the two dimensional quantum confinement along the tube ring direction.

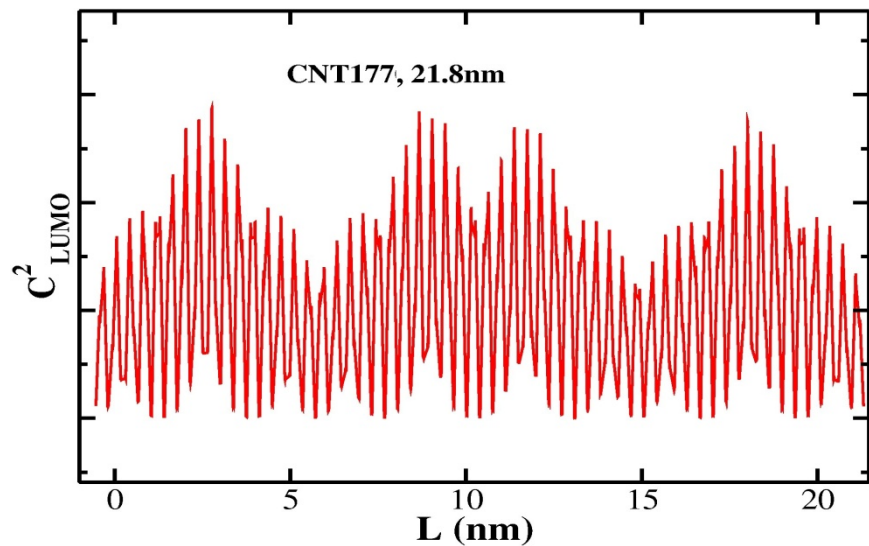
(5, 5) metallic CNT

DFT
B3LYP/6-31G

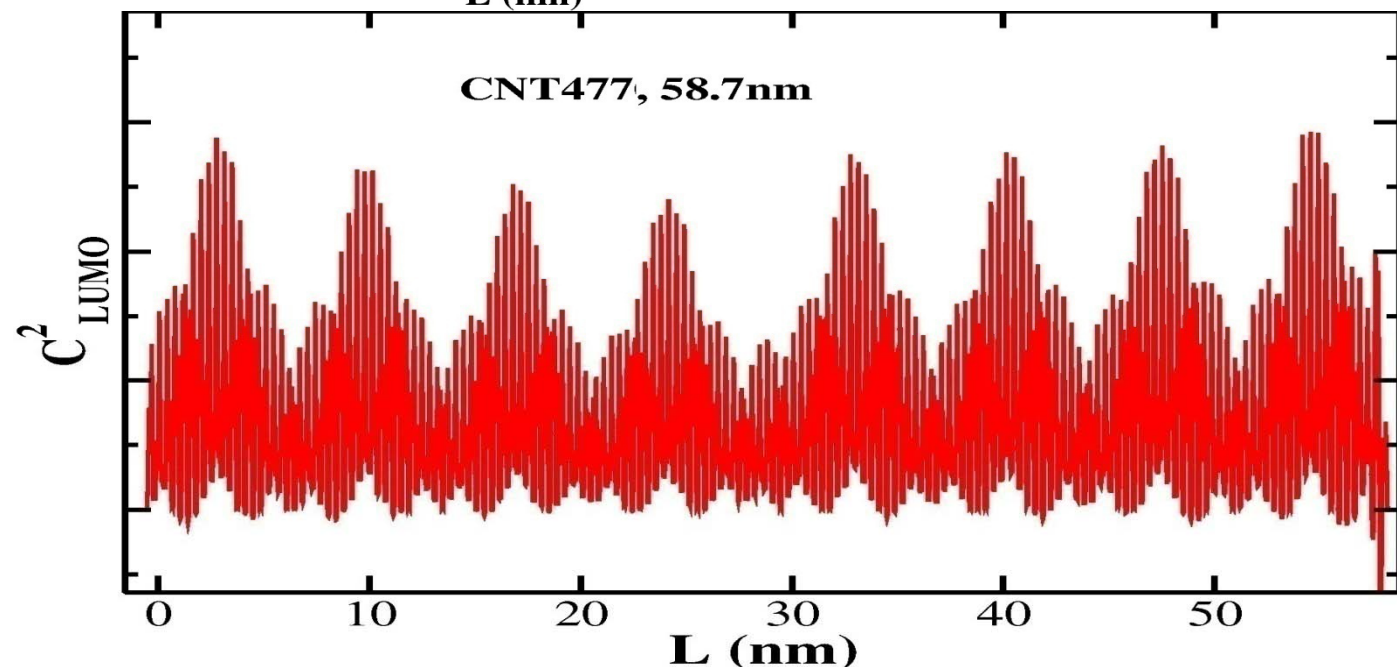
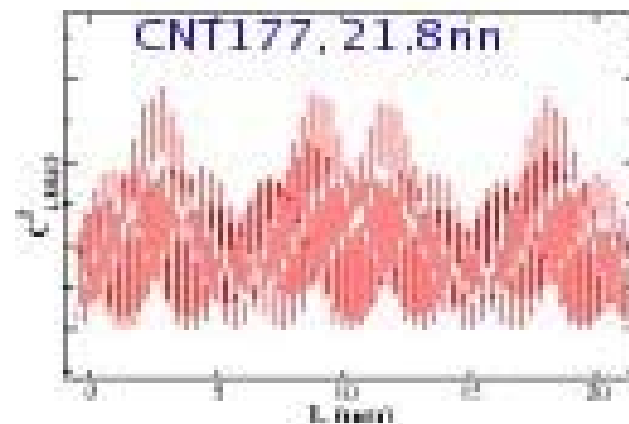
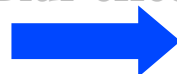


(5, 5) metallic CNT

1D Wavefunction along tube direction



Blur effect



$T(w)=36$ layer

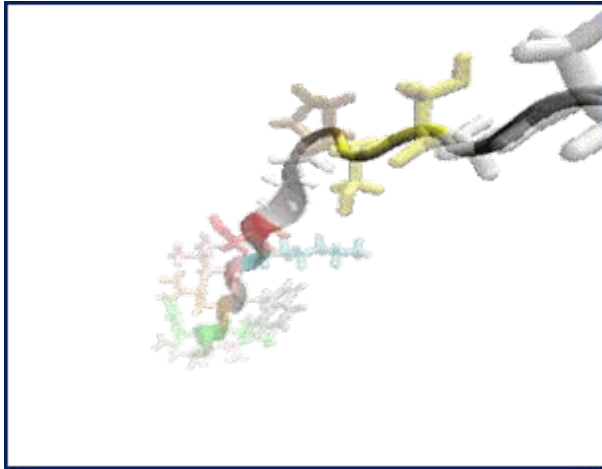
- **CIS calculation provide accurate electronic structures for very long CNT**
- **CIS found bloch-alike wavefunction in CNT without assuming any periodical boundary conditions.**

分子光子学的多尺度理论研究

究

分子光子学：分子科学和物理科学交叉，识别和操纵分子与光子的相互作用，探测结构变化并从分子角度理解现象

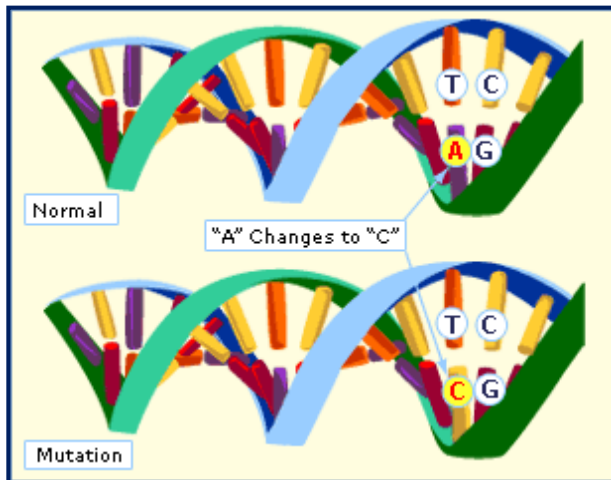
蛋白质折叠



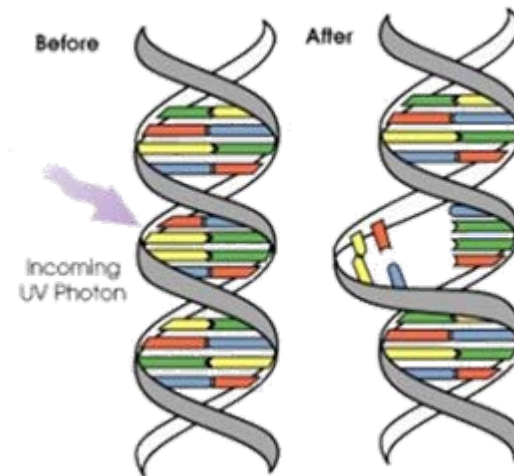
蛋白质聚合



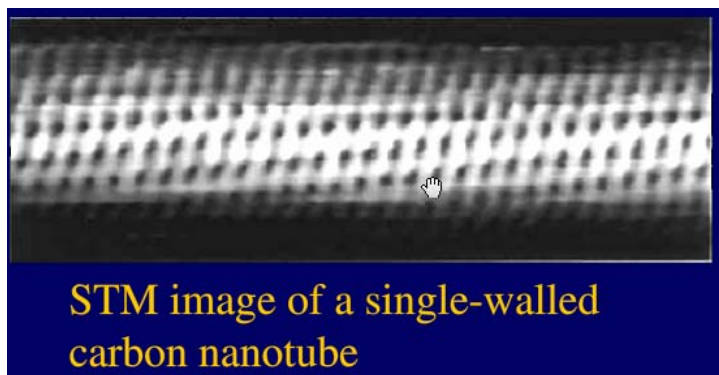
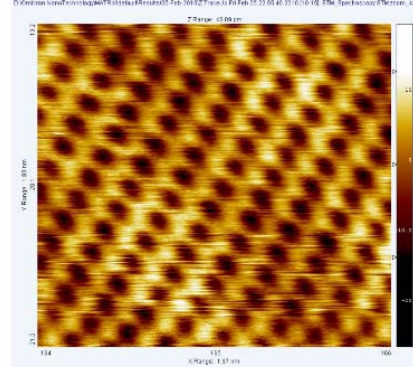
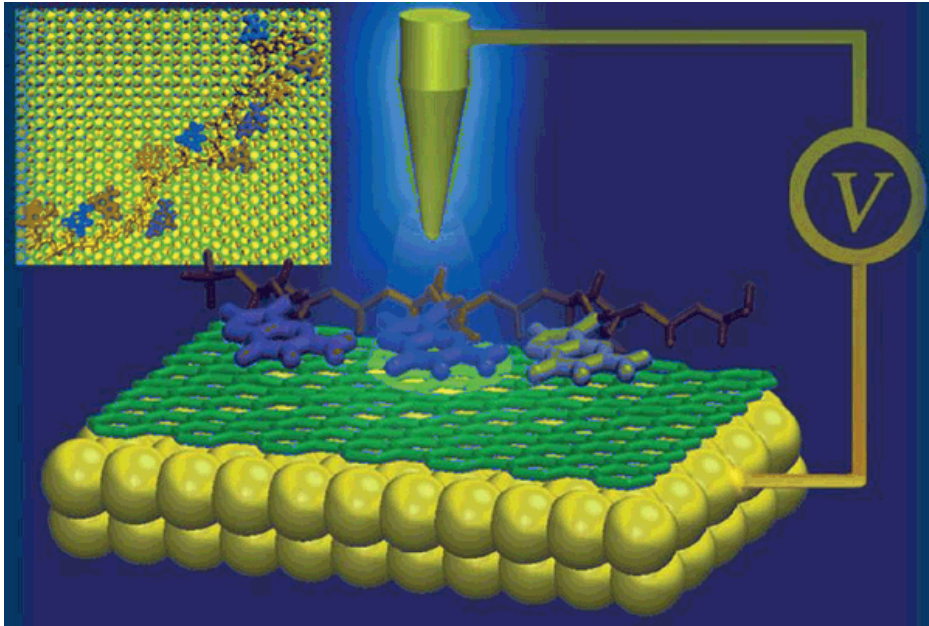
DNA突变改变蛋白



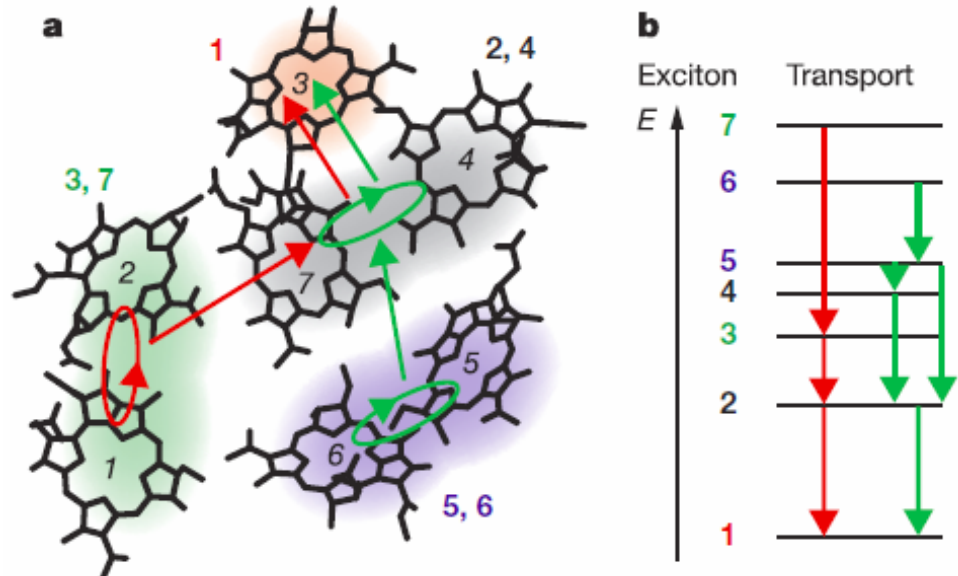
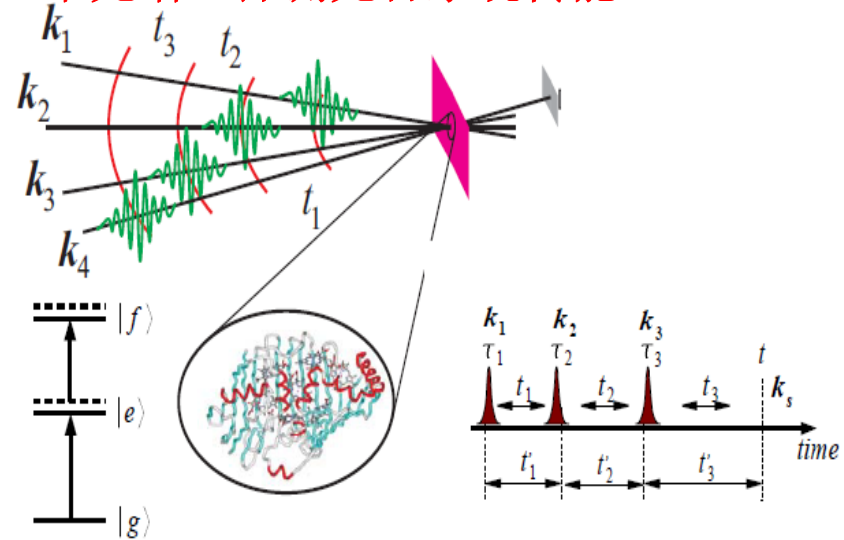
DNA紫外损伤



➤ 扫描隧道显微镜 (STM) : 探测材料微观结构



➤ 二维光谱: 探测光合系统传能



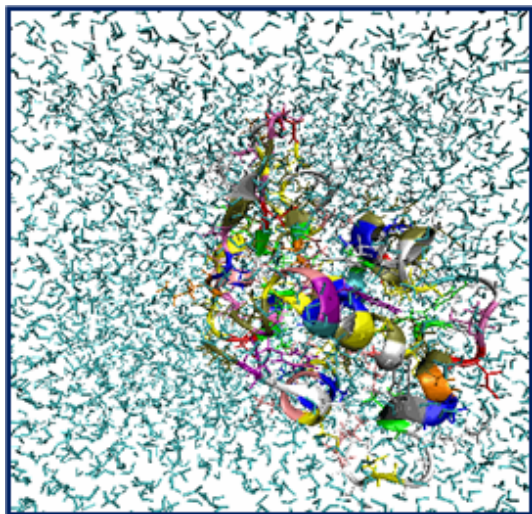
Graham Fleming, Tobias Brixner, Berkeley

多尺度模拟处理环境涨落中大分子宏观性能

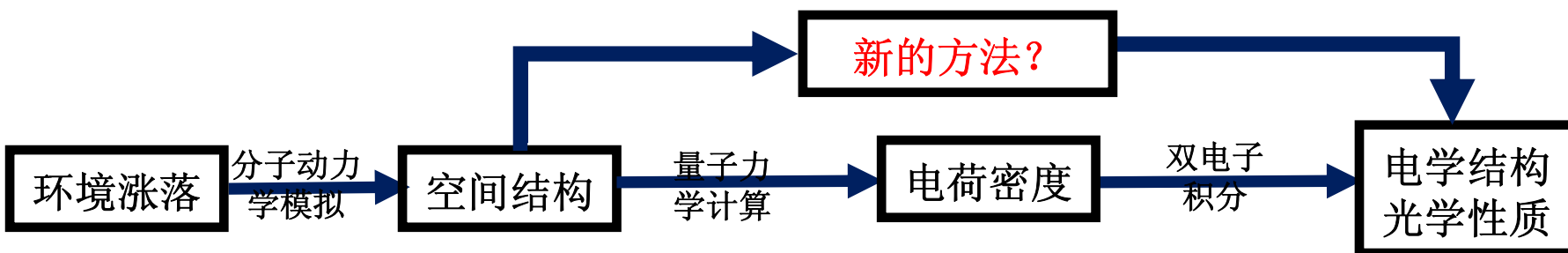
我们的工作:

- 开发EHEF (Exciton Hamiltonian with Electrostatic Fluctuations) 算法有效结合量子力学 (表征小分子片段) 和分子动力学 (描述生物大分子和环境) 模拟
- 为光谱计算软件SPECTRON开发EHEF模块, 研究生物大分子的多维光谱特征
- 发掘生物功能的化学与物理机理, 测量和预估生物分子的功能属性

生物分子的环境涨落为光谱理论研究带来挑战！

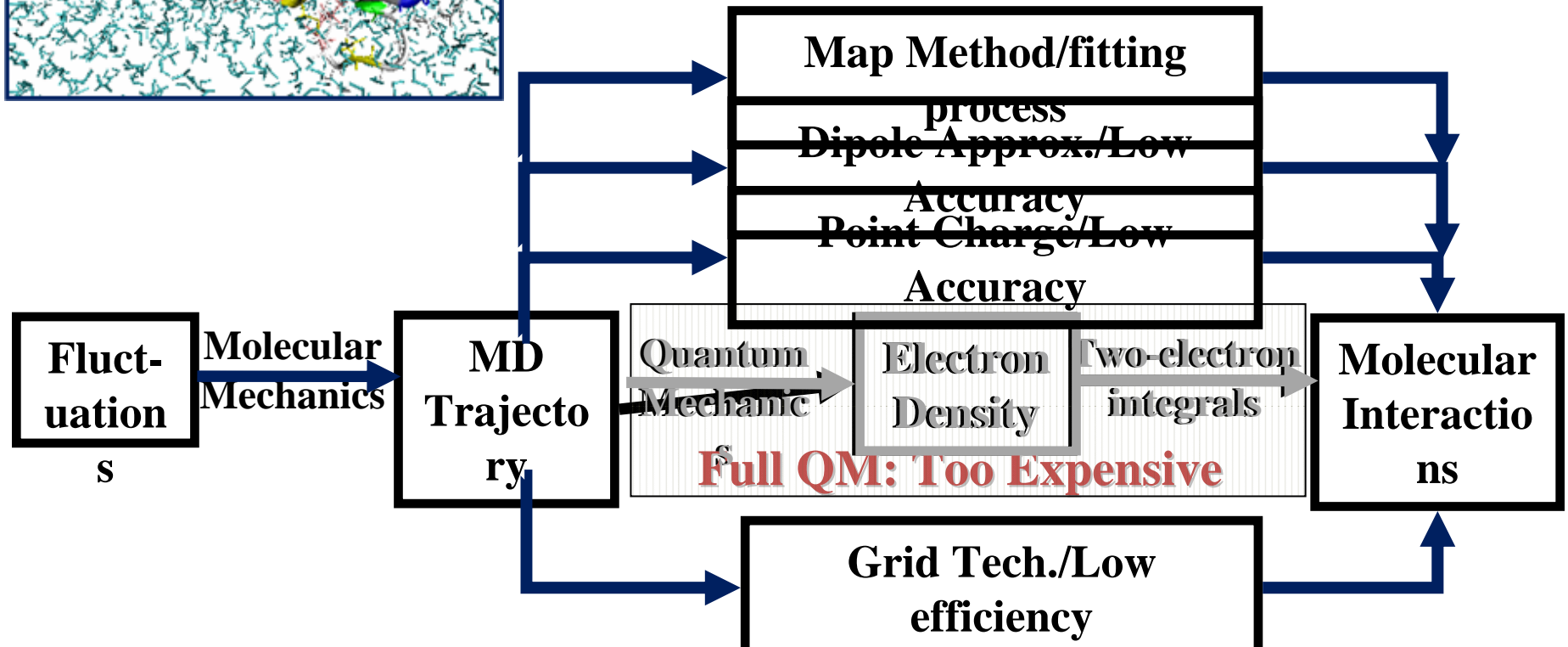
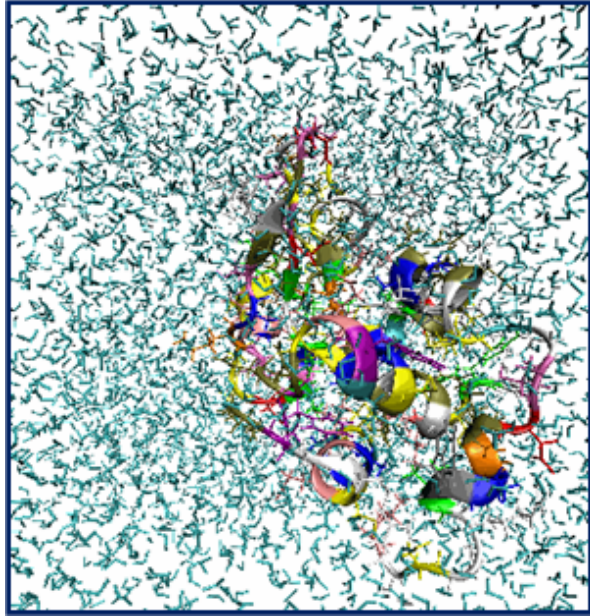


- 环境涨落引起结构变化需要大量分子动力学快照描述
- 光学性质模拟要求对所有动态快照进行量子力学计算
- 现有计算能力无法实现**多次量子力学和双电子积分计算**



Challenge for theoretical study

Fluctuations of proteins and environment: Change spectral features



Map method for environmental fluctuations

Energy of a state can be expressed as

$$E = E_0 - \mu \cdot F$$

Map for excitation energy are constructed by

$$\varepsilon_m^F = \varepsilon_m + \sum_i \alpha_i \mathbf{F}_i + \sum_i \beta_i \frac{d\mathbf{F}_i}{dr} + \dots$$

or

$$\varepsilon_m^F = \varepsilon_m + \sum_i \alpha'_i \mathbf{K}_i + \sum_i \beta'_i \mathbf{K}_i^2 + \dots$$

Advantages: Cheap computation costs & Easy to test
--successful utilizations in 2DIR studies

Disadvantages:

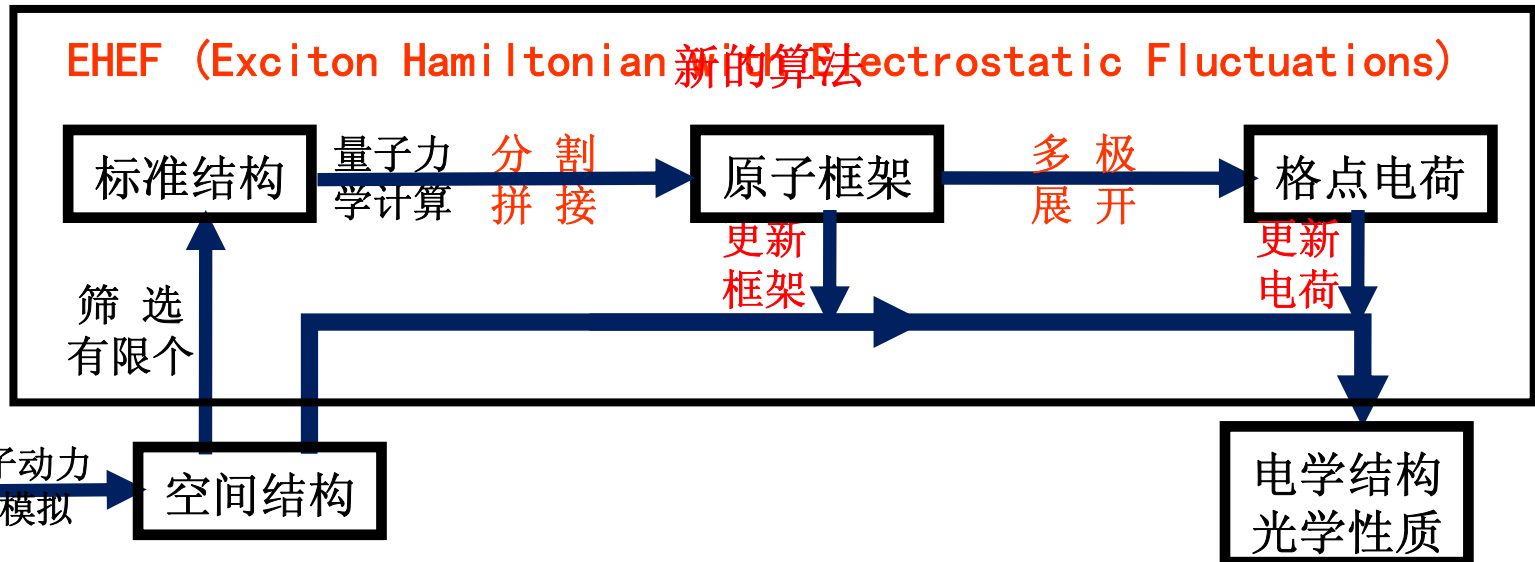
Rely on many QM calculations and heavy analysis

Fitted parameters are not transferable

Lack of predict power

发展新算法实现环境涨落过程的量子力学描述

- 基于**分割拼接**原理，在演化中使用原子框架电荷密度，**避免多次量子力学计算**
- 应用**多极展开**原理，**转换昂贵的双电子积分为廉价的点电荷相互作用计算**
- EHEF (环境涨落激子哈密顿) 算法实现大量分子动力学快照的高速量子力学计算，为生物体系**微观性质的宏观集成模拟**提供了新思路



Jiang, and Mukamel, *Phys. Chem. Chem. Phys.*, **13**, 2394 (2011)

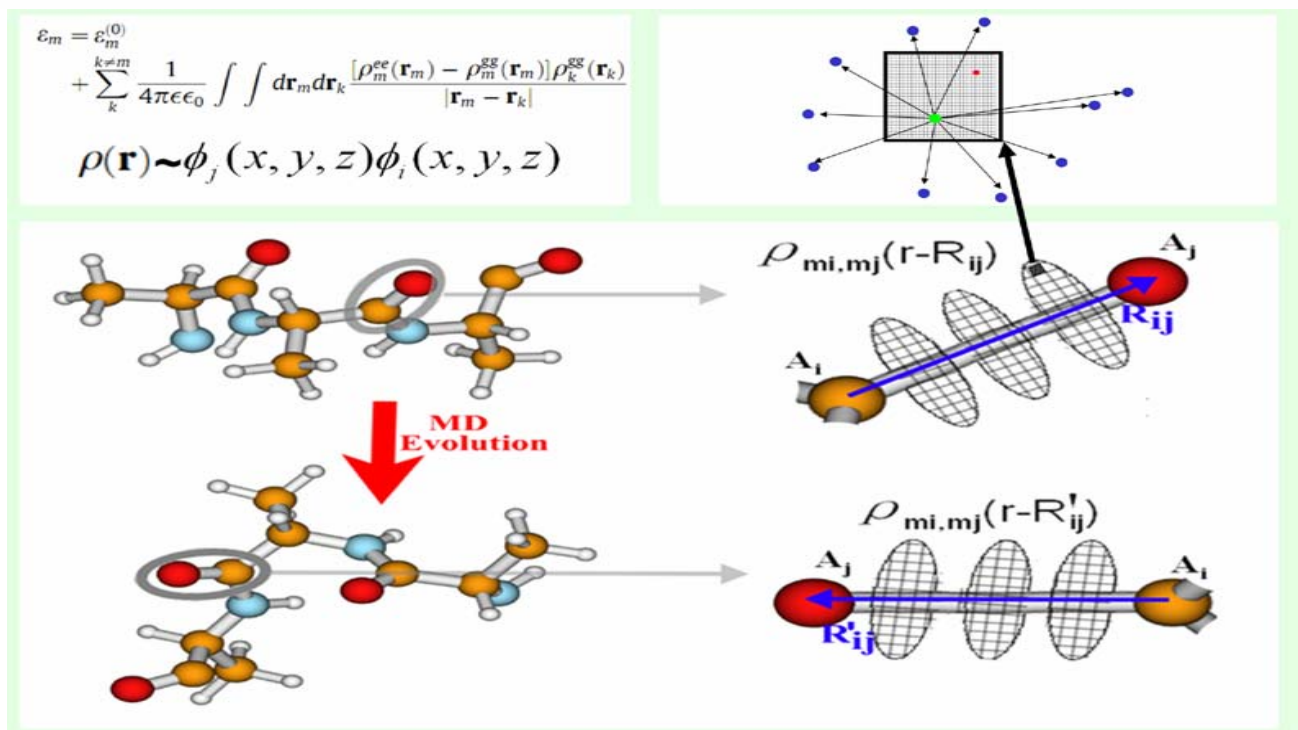
Jiang, Abramavicius, *et. al.* *J. Phys. Chem. B.* **114**, 8270 (2010)

Abramavicius, Jiang, *et. al.* *J. Am. Chem. Soc.* **132**, 7769 (2010)

EHEF (Exciton Hamiltonian with Electrostatic Fluctuations) algorithm

EHEF, uses a limited number of charge grids to produce the same local electrostatic potential as that induced by charge density, and converts the integration of charge density to the product of two charge grids. It avoids repeated QM studies and calculates interactions with low cost, so that it efficiently constructs a QM-based exciton Hamiltonian for thousands of MM snapshots.

$$\frac{1}{4\pi\epsilon\epsilon_0} \int \int d\mathbf{r}_m d\mathbf{r}_k \frac{[\rho_m^{ee}(\mathbf{r}_m) - \rho_m^{gg}(\mathbf{r}_m)]\rho_k^{gg}(\mathbf{r}_k)}{|\mathbf{r}_m - \mathbf{r}_k|} \cong \sum_{ij} \frac{M_m^{eg}(i) M_k^{gg}(j)}{4\pi\epsilon_0 r_{ij}}$$



EHEF (Exciton Hamiltonian with Electrostatic Fluctuations) algorithm

1. Define atomic frame for each pair of atoms, $(\mathbf{R}, \theta, \gamma)$

2. Calculations involve charge densities (As expensive as calculating 2-e integrals)

3. To obtain low computation cost, use a limited number of large grids (10^3 for an amino acid).

4. Each Grid is divided into a large number of sub-grids (10^6 for an amino acid), to maintain the same precision as 2-e integrals.

5. Electrostatic potentials at random sample positions are calculated from charges in 10^3 sub-grids, and are used to fit one point charge for one grid.

6. Charge distributions are saved in the atomic frame.

7. Assume fixed charge distribution in the atomic frame

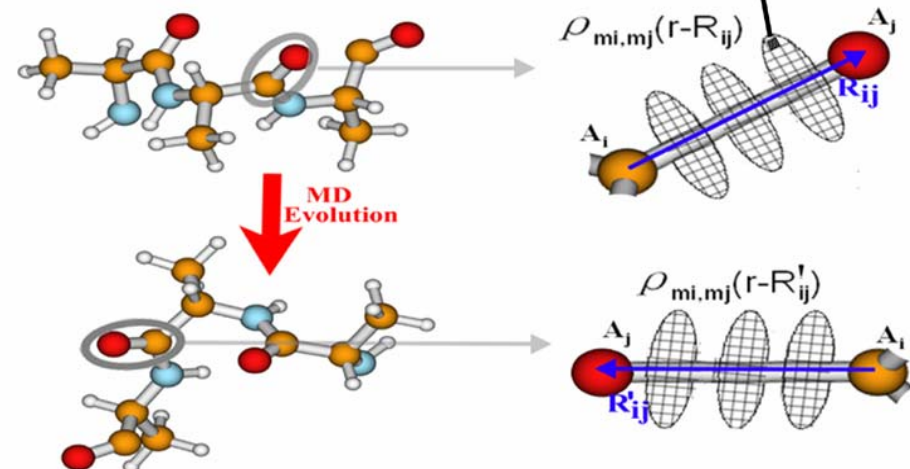
8. Update the new atomic frame during MD evolutions $(\mathbf{R}', \theta', \gamma')$

9. Update the charge density in the new atomic frame.

10. Calculate energy shift due to fluctuations.

$$\epsilon_m = \epsilon_m^{(0)} + \sum_k \frac{1}{4\pi\epsilon\epsilon_0} \int \int d\mathbf{r}_m d\mathbf{r}_k \frac{[\rho_m^{ee}(\mathbf{r}_m) - \rho_m^{gg}(\mathbf{r}_m)]\rho_k^{gg}(\mathbf{r}_k)}{|\mathbf{r}_m - \mathbf{r}_k|}$$

$$\rho(\mathbf{r}) \sim \phi_j(x, y, z)\phi_i(x, y, z)$$



J. Jiang, D. Abramavicius, S. Mukamel, J. Phys. Chem. B. 2010, 114, 8270

J. Jiang, S. Mukamel, Phys. Chem. Chem. Phys. 2011, 13, 2394

EHEF (Exciton Hamiltonian with Electrostatic Fluctuations) algorithm

- ❖ **Accurate -- calculations without fitting parameters**
- ❖ **Efficient -- Atomic frame to avoid repeated QM studies, Grid charge fitted from electrostatic potential avoid integrations**
- ❖ **Transferable for different systems and applications**
- ❖ **Able to explain experiments and predict new information**

蛋白质的淀粉样纤维沉积

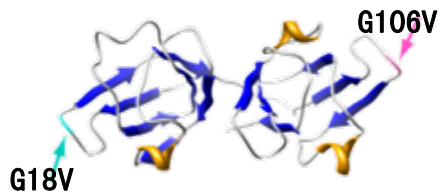


多种疾病和蛋白质的淀粉样纤维的沉积有关，
包括阿尔兹海默病、帕金森病、可传播性海绵状脑病；

重大难题：

- 没有合适的观察测量技术，传统的X-ray，NMR，CD等不适用
- 纤维堆积的驱动原因和过程不清楚
- 蛋白质发生纤维堆积的能力无法测量和预估

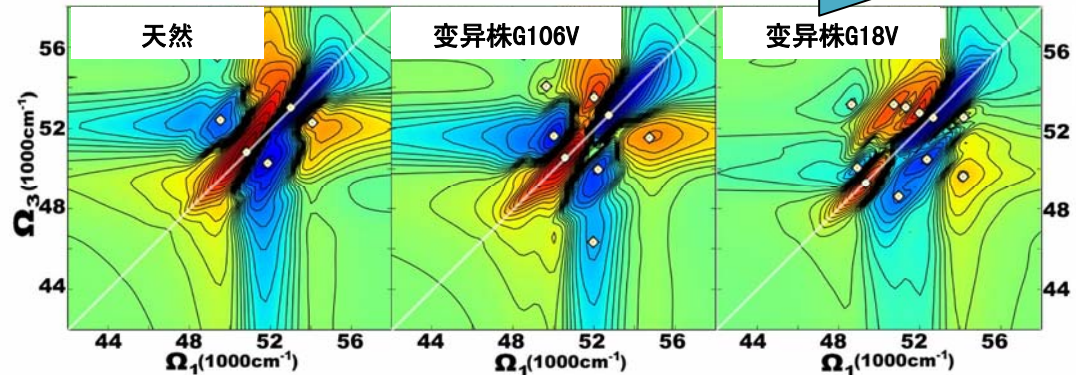
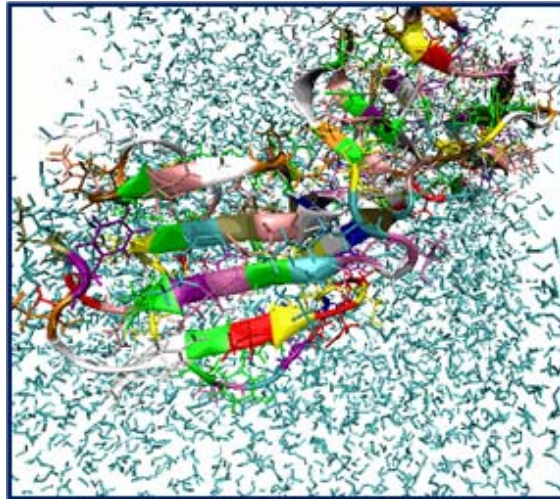
应用二维紫外光谱给出了答案



蛋白质 γ S-crystallin 的两种变异株 G18V 和 G106V 发生纤维堆积可导致人眼白内障

二维光谱信号近似熵(复杂度)

0.66 < 0.71 < 0.75



纤维堆积能力

理论预测被 Rachel Martin 教授实验验证 (Biophys. J., 100, 498 (2011))
进一步预测成功 14 种蛋白质的纤维堆积能力

二维光谱帮助淀粉样纤维堆积的研究走出困境:

- 提供可观测蛋白结构和序列变化的**特征谱**
- 提出可测量、可计算、可数值化的**纤维堆积能力指标**
- 发现**物理机理**: 纤维堆积的驱动力即生物系统降低熵的倾向

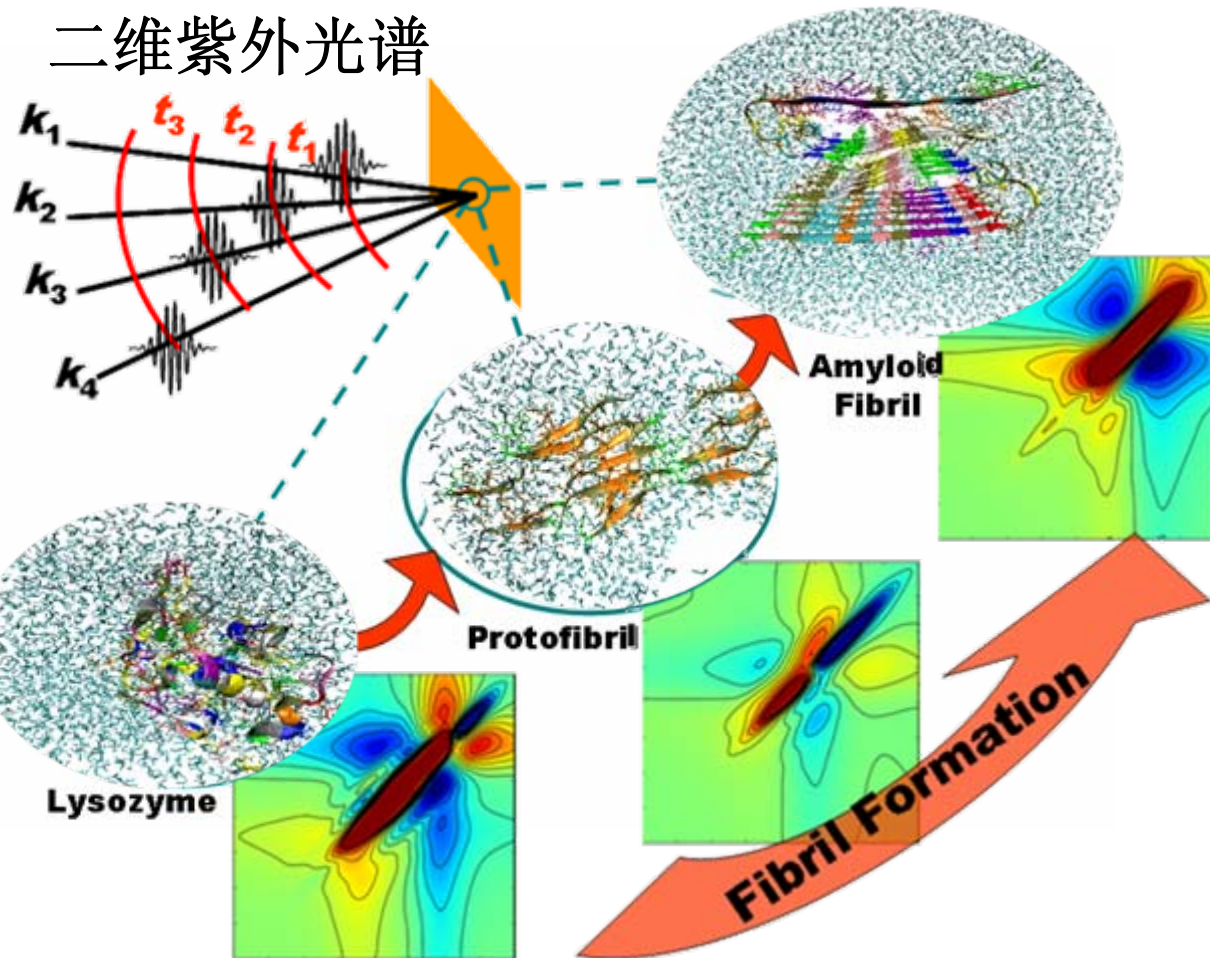
Jiang, and Mukamel, Angew. Chem. Int. Ed. 49, 9666 (2010)

应用QM/MM模拟二维紫外光谱研究蛋白质结构与功能关系

多种疾病(阿尔兹海默病、帕金森病)和蛋白质的淀粉样纤维的沉积有关

重大难题

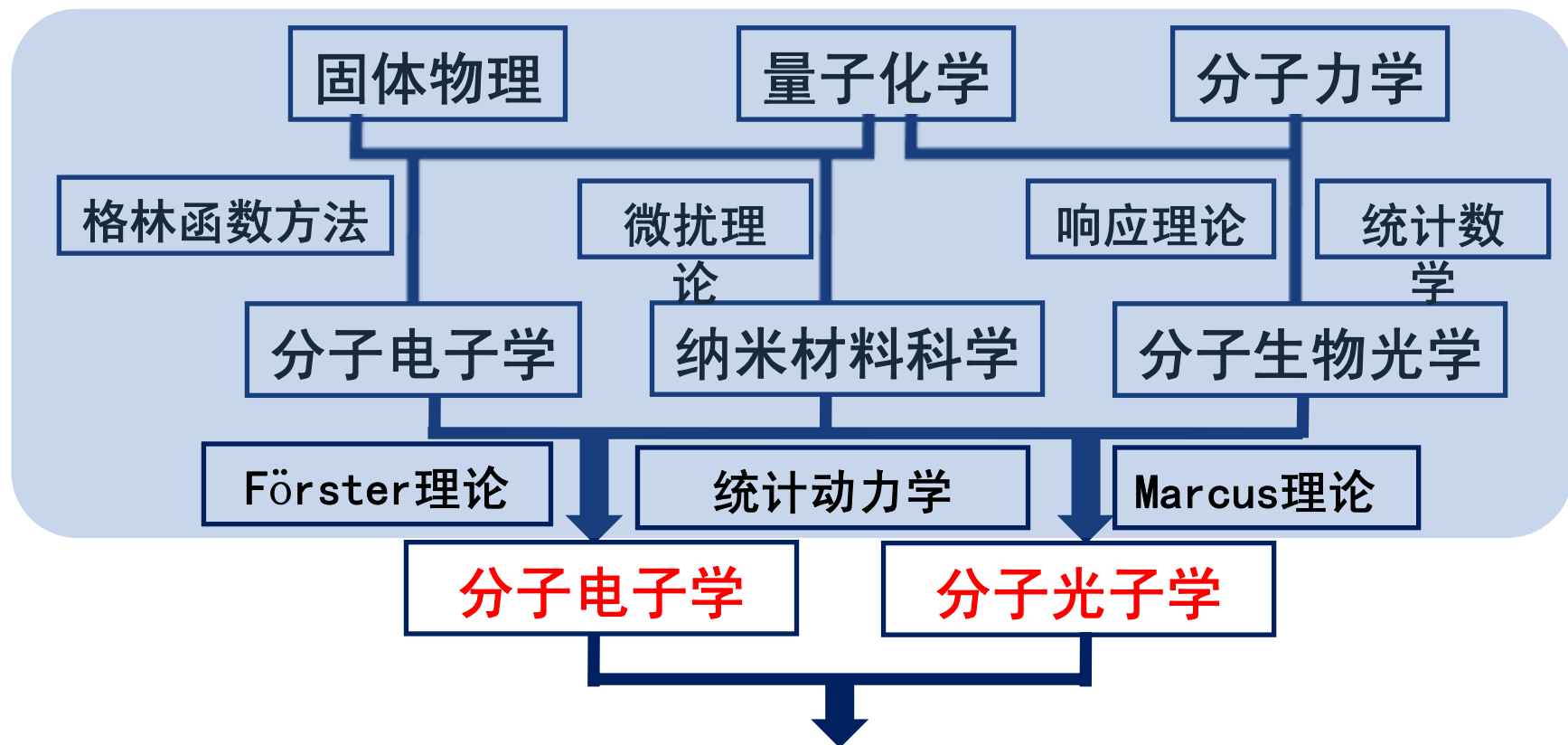
- 没有合适的观察测量技术, 传统的X-ray, NMR, CD等不适用
- 纤维堆积的驱动原因和过程不清楚



二维光谱帮助淀粉样纤维堆积的研究走出困境:

- 提供可观测蛋白结构和序列变化的**特征谱**
- 提出可测量、可计算的**纤维堆积能力指标**
- 发现**物理机理**: 纤维堆积的驱动力即生物系统降低熵的倾向

多尺度研究



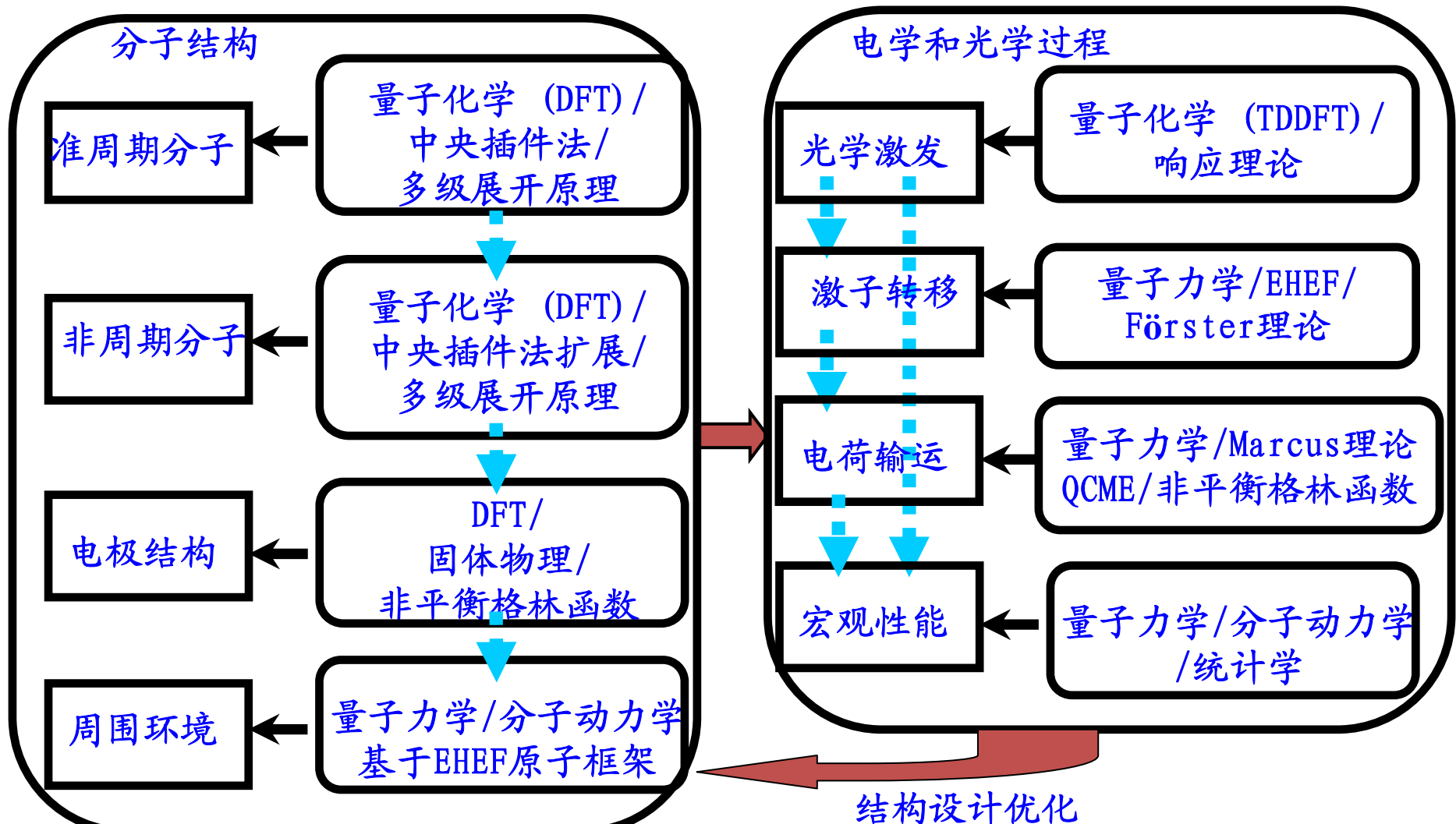
- 远期学术目标：发展基于第一性原理的**多尺度理论方法及高效计算软件**
- 研究目的：发掘分子体系结构与功能在物理和化学上的**新现象与新机理**
- 应用出口：为分子技术发展提供**新原理、新方法和新途径**

展望

- 发展多尺度模拟成为**潮流**：世界上很多优秀研究组 (Goddard:Caltech, Martinez:Stanford, Steinhauser:Fraunhofer等等)都在努力
- 多尺度模拟计算软件很可能承继四十年前的 Gaussian70 (98年诺贝尔奖) 和九十年代的量化软件大潮，呈现以二十年为周期的计算化学**飞跃**
- 麻省理工Sidney Yip教授：“多尺度模拟的前沿正在迅速扩展，前景广阔，但**挑战**仍然巨大，年轻学者可以大有作为”。
- 致力于为我国在多尺度方法发展及软件开发方面做出一些**贡献**

发展多尺度的理论框架

- 针对真实体系的复杂性，有机结合量子化学、分子动力学、固体物理、响应理论等方法，模拟纳米材料和生物大分子系统在各种空间和时间尺度下的系统和效应
- 开发计算软件，集成微观机理构筑宏观效应，提供结构、功能和机理等关键信息



致谢

中国科学院上海技术物理研究所

陆卫 研究员

李宁 研究员

瑞典皇家工学院 (Royal Institute of Technology, Sweden)

罗毅 教授

Hans Agren 教授

高斌 博士

曹辉 博士

美国加州大学尔湾分校 (University of California, Irvine)

Prof. Shaul Mukamel

Dr. Darius Abramavicius

Dr. Daniel Healion

Dr. Lijun Yang

谢谢各位！